Heller Ehrman White & McAuliffe, LLP
Title: Use of Computationally Derived Protein Structures of Genetic
Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
Serial No.: 09/709,905   Applicants: Ramnarayan *et al.*
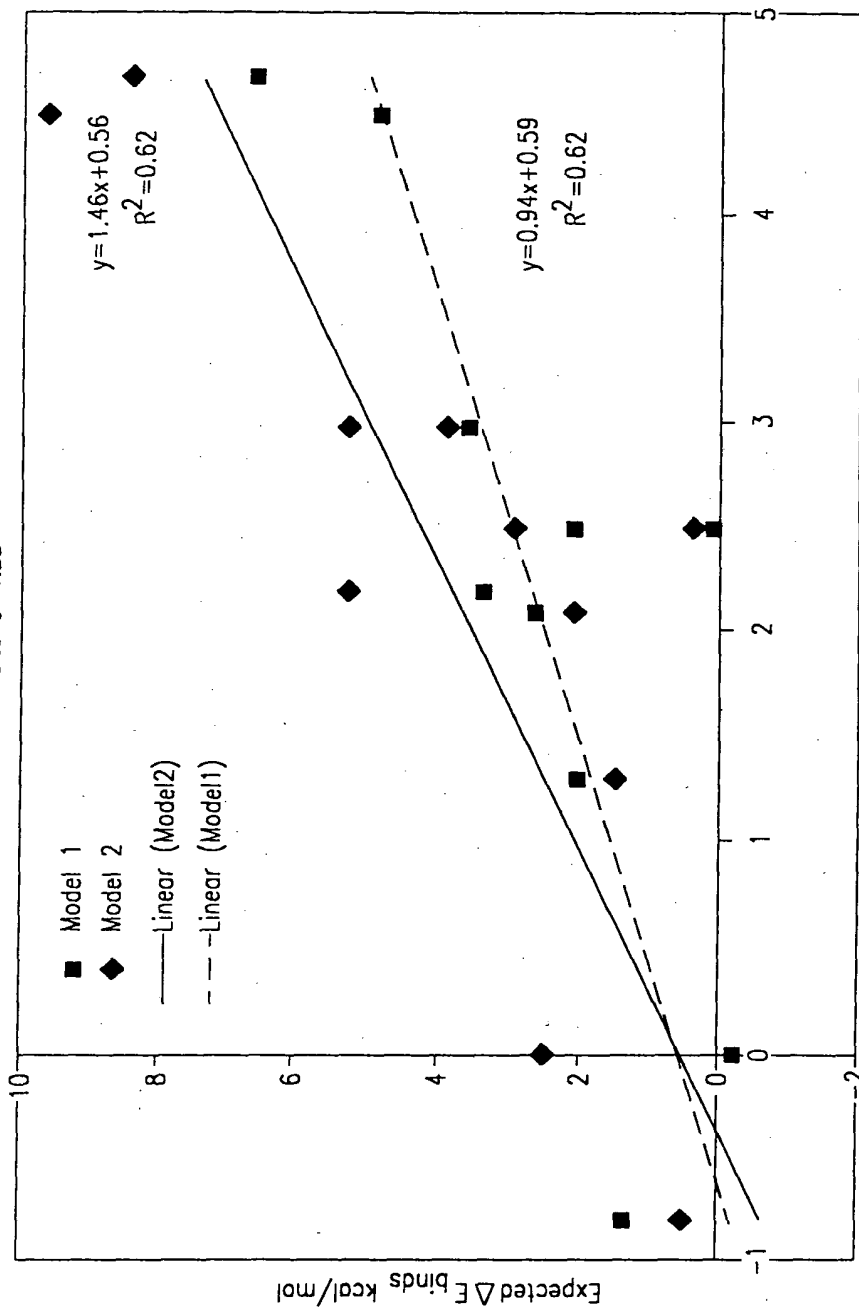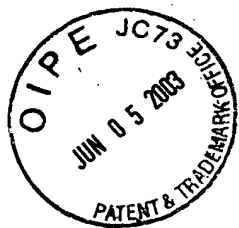Filed: 11/10/00   Attorney Docket No. 24737-1906C

Correlation between Experimental and Calculated Changes
of Binding Energy upon Ligand Modifications in the Binding
Site of NS3

- ■ Model 1
- ◆ Model 2
- —— Linear (Model2)
- — — Linear (Model1)

$y = 1.46x + 0.56$
$R^2 = 0.62$

$y = 0.94x + 0.59$
$R^2 = 0.62$

Expected ΔE_{binds} kcal/mol

Expected ΔE_{binds} kcal/mol

FIG. 4

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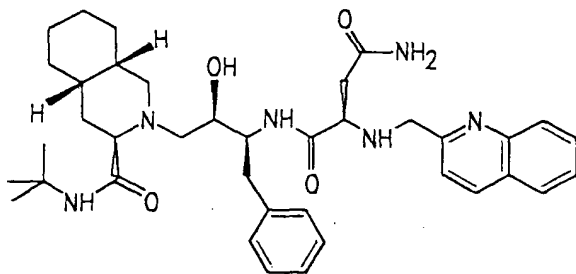Sheet 2 of 33
Title: Use of Computationally Derived Protein Structures of Genetic
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HIV PROTEASE INHIBITORS APPROVED BY FDA

SAQUINAVIR

NELFINAVIR
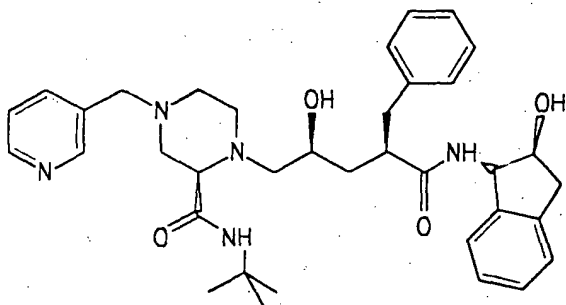
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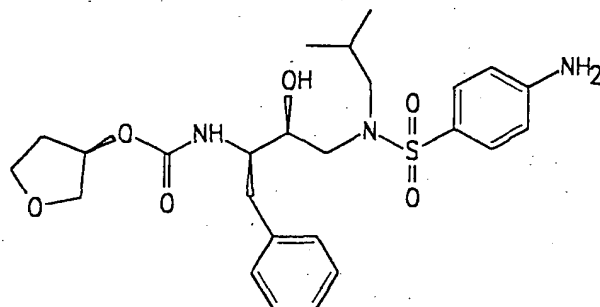
AMPRENAVIR
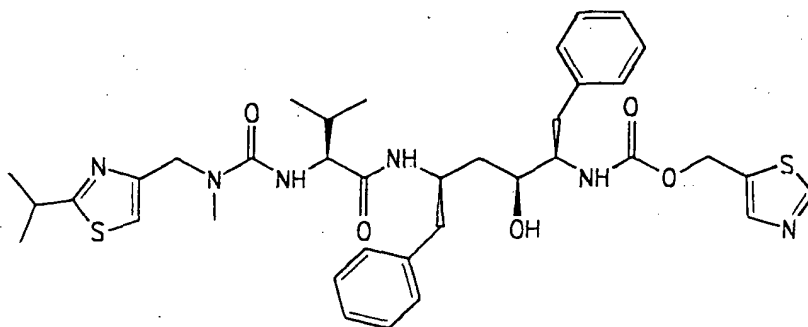
RITONAVIR

FIG. 6
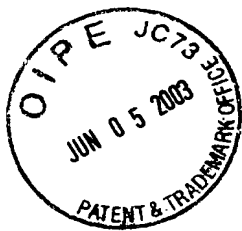
Heller Ehrman White & McAuliffe, LLP
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Title: Use of Computationally Derived Protein Structures of Genetic
Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
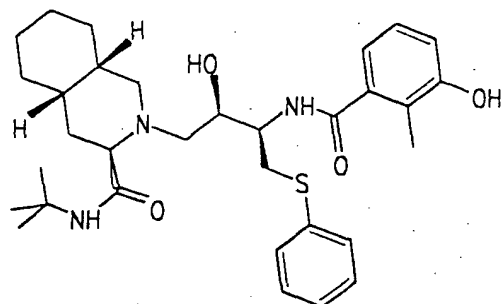Serial No.: 09/709,905   Applicants: Ramnarayan *et al.*
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FIG. 7

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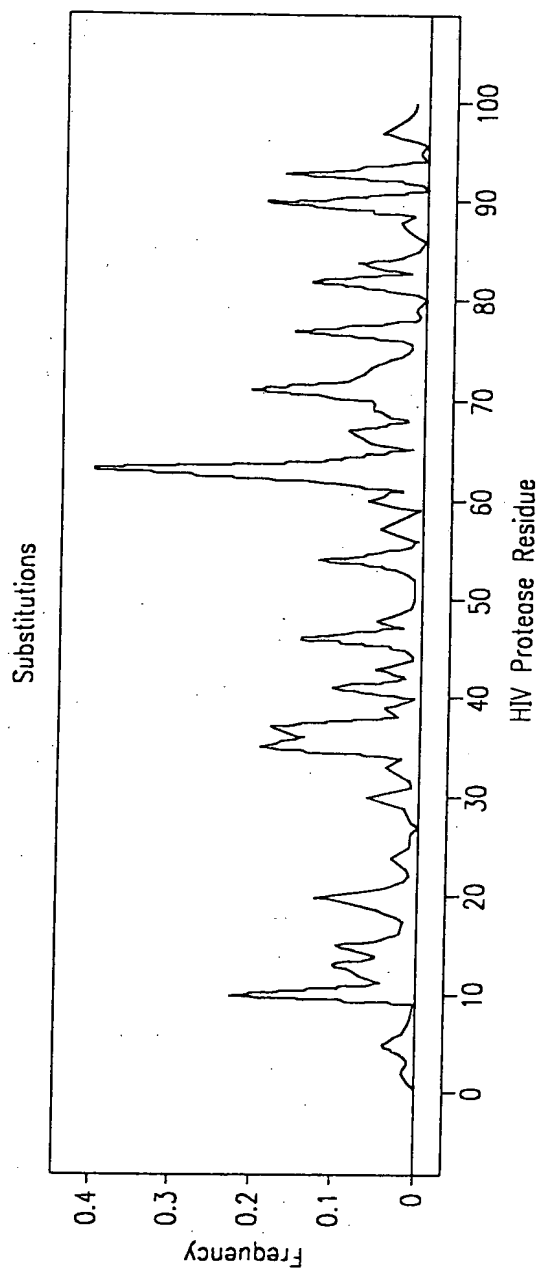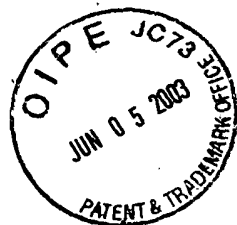Filed: 11/10/00   Attorney Docket No. 24737-1906C

| | | | | | | | | |
|------|----|-----|---|---|---------|--------|--------|
| ATOM | 1 | N | PRO | A | 1 | -3.433 | 7.956 | 34.152 |
| ATOM | 2 | CA | PRO | A | 1 | -2.653 | 6.918 | 34.784 |
| ATOM | 3 | C | PRO | A | 1 | -1.242 | 7.005 | 34.259 |
| ATOM | 4 | O | PRO | A | 1 | -0.950 | 7.638 | 33.216 |
| ATOM | 5 | CB | PRO | A | 1 | -3.281 | 5.601 | 34.262 |
| ATOM | 6 | CG | PRO | A | 1 | -4.191 | 5.995 | 33.118 |
| ATOM | 7 | CD | PRO | A | 1 | -4.547 | 7.461 | 33.339 |
| ATOM | 8 | 1H | PRO | A | 1 | -2.845 | 8.493 | 33.547 |
| ATOM | 9 | 2H | PRO | A | 1 | -3.824 | 8.552 | 34.853 |
| ATOM | 10 | N | GLN | A | 2 | -0.259 | 6.464 | 35.001 |
| ATOM | 11 | H | GLN | A | 2 | -0.475 | 6.057 | 35.889 |
| ATOM | 12 | CA | GLN | A | 2 | 1.115 | 6.443 | 34.568 |
| ATOM | 13 | C | GLN | A | 2 | 1.452 | 4.993 | 34.301 |
| ATOM | 14 | O | GLN | A | 2 | 1.379 | 4.106 | 35.173 |
| ATOM | 15 | CB | GLN | A | 2 | 2.070 | 6.966 | 35.653 |
| ATOM | 16 | CG | GLN | A | 2 | 3.549 | 6.859 | 35.240 |
| ATOM | 17 | CD | GLN | A | 2 | 4.490 | 7.744 | 36.054 |
| ATOM | 18 | OE1 | GLN | A | 2 | 4.771 | 8.888 | 35.719 |
| ATOM | 19 | NE2 | GLN | A | 2 | 4.980 | 7.190 | 37.144 |
| ATOM | 20 | 1HE2 | GLN | A | 2 | 5.605 | 7.702 | 37.734 |
| ATOM | 21 | 2HE2 | GLN | A | 2 | 4.731 | 6.253 | 37.390 |
| ATOM | 22 | N | ILE | A | 3 | 1.784 | 4.644 | 33.037 |
| ATOM | 23 | H | ILE | A | 3 | 1.876 | 5.351 | 32.336 |
| ATOM | 24 | CA | ILE | A | 3 | 2.013 | 3.257 | 32.665 |
| ATOM | 25 | C | ILE | A | 3 | 3.505 | 3.028 | 32.473 |
| ATOM | 26 | O | ILE | A | 3 | 4.242 | 3.777 | 31.787 |
| ATOM | 27 | CB | ILE | A | 3 | 1.226 | 2.944 | 31.370 |
| ATOM | 28 | CG1 | ILE | A | 3 | -0.274 | 3.239 | 31.603 |
| ATOM | 29 | CG2 | ILE | A | 3 | 1.427 | 1.480 | 30.901 |
| ATOM | 30 | CD1 | ILE | A | 3 | -1.089 | 3.219 | 30.322 |
| ATOM | 31 | N | THR | A | 4 | 4.071 | 2.032 | 33.177 |
| ATOM | 32 | H | THR | A | 4 | 3.525 | 1.525 | 33.844 |
| ATOM | 33 | CA | THR | A | 4 | 5.451 | 1.661 | 33.007 |
| ATOM | 34 | C | THR | A | 4 | 5.515 | 0.637 | 31.901 |
| ATOM | 35 | O | THR | A | 4 | 4.490 | 0.143 | 31.397 |
| ATOM | 36 | CB | THR | A | 4 | 6.051 | 1.125 | 34.324 |
| ATOM | 37 | OG1 | THR | A | 4 | 5.224 | 0.069 | 34.791 |
| ATOM | 38 | HG1 | THR | A | 4 | 5.589 | -0.299 | 35.646 |
| ATOM | 39 | CG2 | THR | A | 4 | 6.085 | 2.212 | 35.431 |
| ATOM | 40 | N | LEU | A | 5 | 6.677 | 0.281 | 31.405 |
| ATOM | 41 | H | LEU | A | 5 | 7.518 | 0.530 | 31.885 |
| ATOM | 42 | CA | LEU | A | 5 | 6.754 | -0.464 | 30.177 |
| ATOM | 43 | C | LEU | A | 5 | 7.432 | -1.813 | 30.356 |
| ATOM | 44 | O | LEU | A | 5 | 7.940 | -2.464 | 29.426 |
| ATOM | 45 | CB | LEU | A | 5 | 7.459 | 0.394 | 29.128 |
| ATOM | 46 | CG | LEU | A | 5 | 6.668 | 1.671 | 28.775 |
| ATOM | 47 | CD1 | LEU | A | 5 | 7.493 | 2.649 | 27.939 |
| ATOM | 48 | CD2 | LEU | A | 5 | 5.345 | 1.307 | 28.099 |
| ATOM | 49 | N | TRP | A | 6 | 7.420 | -2.351 | 31.594 |
| ATOM | 50 | H | TRP | A | 6 | 7.030 | -1.833 | 32.356 |
| ATOM | 51 | CA | TRP | A | 6 | 7.958 | -3.669 | 31.865 |
| ATOM | 52 | C | TRP | A | 6 | 7.071 | -4.697 | 31.204 |
| ATOM | 53 | O | TRP | A | 6 | 7.520 | -5.798 | 30.828 |
| ATOM | 54 | CB | TRP | A | 6 | 8.099 | -3.913 | 33.367 |
| ATOM | 55 | CG | TRP | A | 6 | 9.041 | -2.974 | 34.070 |

FIG. 11

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ATOM	56	CD1	TRP	A	6	8.745	-1.769	34.646
ATOM	57	CD2	TRP	A	6	10.449	-3.171	34.273
ATOM	58	NE1	TRP	A	6	9.875	-1.209	35.190
ATOM	59	HE1	TRP	A	6	9.930	-0.332	35.668
ATOM	60	CE2	TRP	A	6	10.932	-2.048	34.974
ATOM	61	CE3	TRP	A	6	11.334	-4.190	33.924
ATOM	62	CZ2	TRP	A	6	12.257	-1.917	35.333
ATOM	63	CZ3	TRP	A	6	12.650	-4.065	34.278
ATOM	64	CH2	TRP	A	6	13.106	-2.942	34.974
ATOM	65	N	GLN	A	7	5.773	-4.448	30.973
ATOM	66	H	GLN	A	7	5.354	-3.619	31.343
ATOM	67	CA	GLN	A	7	4.952	-5.339	30.205
ATOM	68	C	GLN	A	7	4.438	-4.569	29.033
ATOM	69	O	GLN	A	7	4.433	-3.321	29.000
ATOM	70	CB	GLN	A	7	3.712	-5.693	30.969
ATOM	71	CG	GLN	A	7	4.015	-6.467	32.210
ATOM	72	CD	GLN	A	7	2.734	-6.678	32.917
ATOM	73	OE1	GLN	A	7	2.053	-7.681	32.712
ATOM	74	NE2	GLN	A	7	2.356	-5.682	33.736
ATOM	75	1HE2	GLN	A	7	1.501	-5.748	34.251
ATOM	76	2HE2	GLN	A	7	2.926	-4.867	33.837
ATOM	77	N	ARG	A	8	3.777	-5.239	28.078
ATOM	78	H	ARG	A	8	3.688	-6.233	28.142
ATOM	79	CA	ARG	A	8	3.183	-4.568	26.948
ATOM	80	C	ARG	A	8	2.117	-3.648	27.461
ATOM	81	O	ARG	A	8	1.333	-3.965	28.387
ATOM	82	CB	ARG	A	8	2.574	-5.555	25.975
ATOM	83	CG	ARG	A	8	3.532	-6.593	25.437
ATOM	84	CD	ARG	A	8	2.842	-7.610	24.579
ATOM	85	NE	ARG	A	8	3.787	-8.487	23.900
ATOM	86	HE	ARG	A	8	4.762	-8.279	23.982
ATOM	87	CZ	ARG	A	8	3.405	-9.541	23.185
ATOM	88	NH1	ARG	A	8	2.125	-9.871	23.052
ATOM	89	2HH1	ARG	A	8	1.418	-9.321	23.496
ATOM	90	1HH1	ARG	A	8	1.869	-10.670	22.508
ATOM	91	NH2	ARG	A	8	4.332	-10.286	22.589
ATOM	92	1HH2	ARG	A	8	4.062	-11.082	22.048
ATOM	93	2HH2	ARG	A	8	5.299	-10.050	22.682
ATOM	94	N	PRO	A	9	1.990	-2.428	26.938
ATOM	95	CA	PRO	A	9	1.001	-1.462	27.440
ATOM	96	C	PRO	A	9	-0.365	-1.697	26.821
ATOM	97	O	PRO	A	9	-0.918	-0.935	26.008
ATOM	98	CB	PRO	A	9	1.572	-0.112	27.041
ATOM	99	CG	PRO	A	9	2.553	-0.404	25.931
ATOM	100	CD	PRO	A	9	3.024	-1.820	26.084
ATOM	101	N	LEU	A	10	-1.028	-2.803	27.227
ATOM	102	H	LEU	A	10	-0.616	-3.404	27.912
ATOM	103	CA	LEU	A	10	-2.319	-3.143	26.698
ATOM	104	C	LEU	A	10	-3.390	-2.565	27.591
ATOM	105	O	LEU	A	10	-3.336	-2.632	28.831
ATOM	106	CB	LEU	A	10	-2.451	-4.651	26.709
ATOM	107	CG	LEU	A	10	-1.483	-5.316	25.756
ATOM	108	CD1	LEU	A	10	-1.159	-6.740	26.212
ATOM	109	CD2	LEU	A	10	-2.083	-5.262	24.322
ATOM	110	N	VAL	A	11	-4.447	-1.952	27.033
ATOM	111	H	VAL	A	11	-4.507	-1.875	26.038

FIG. 11A-1
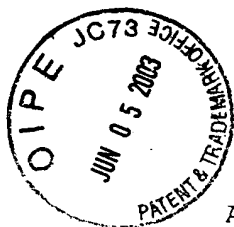
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ATOM	112	CA	VAL	A	11	-5.506	-1.398	27.835
ATOM	113	C	VAL	A	11	-6.827	-1.857	27.268
ATOM	114	O	VAL	A	11	-6.924	-2.490	26.198
ATOM	115	CB	VAL	A	11	-5.420	0.143	27.897
ATOM	116	CG1	VAL	A	11	-4.117	0.595	28.551
ATOM	117	CG2	VAL	A	11	-5.549	0.787	26.497
ATOM	118	N	THR	A	12	-7.954	-1.592	27.978
ATOM	119	H	THR	A	12	-7.884	-1.141	28.868
ATOM	120	CA	THR	A	12	-9.301	-1.942	27.496
ATOM	121	C	THR	A	12	-9.889	-0.726	26.795
ATOM	122	O	THR	A	12	-9.856	0.436	27.247
ATOM	123	CB	THR	A	12	-10.225	-2.385	28.659
ATOM	124	OG1	THR	A	12	-9.596	-3.458	29.338
ATOM	125	HG1	THR	A	12	-10.170	-3.766	30.096
ATOM	126	CG2	THR	A	12	-11.579	-2.895	28.156
ATOM	127	N	ILE	A	13	-10.449	-0.932	25.594
ATOM	128	H	ILE	A	13	-10.409	-1.841	25.178
ATOM	129	CA	ILE	A	13	-11.112	0.133	24.882
ATOM	130	C	ILE	A	13	-12.553	-0.292	24.693
ATOM	131	O	ILE	A	13	-12.935	-1.469	24.821
ATOM	132	CB	ILE	A	13	-10.432	0.364	23.511
ATOM	133	CG1	ILE	A	13	-10.466	-0.896	22.628
ATOM	134	CG2	ILE	A	13	-8.986	0.806	23.747
ATOM	135	CD1	ILE	A	13	-9.755	-0.745	21.294
ATOM	136	N	LYS	A	14	-13.470	0.658	24.438
ATOM	137	H	LYS	A	14	-13.209	1.622	24.481
ATOM	138	CA	LYS	A	14	-14.838	0.330	24.100
ATOM	139	C	LYS	A	14	-15.088	0.877	22.719
ATOM	140	O	LYS	A	14	-14.859	2.059	22.375
ATOM	141	CB	LYS	A	14	-15.855	0.916	25.099
ATOM	142	CG	LYS	A	14	-17.325	0.518	24.864
ATOM	143	CD	LYS	A	14	-18.078	0.146	26.166
ATOM	144	CE	LYS	A	14	-18.826	1.342	26.810
ATOM	145	NZ	LYS	A	14	-19.316	0.929	28.173
ATOM	146	1HZ	LYS	A	14	-19.801	1.693	28.599
ATOM	147	3HZ	LYS	A	14	-18.536	0.670	28.743
ATOM	148	2HZ	LYS	A	14	-19.936	0.150	28.082
ATOM	149	N	ILE	A	15	-15.535	0.005	21.798
ATOM	150	H	ILE	A	15	-15.806	-0.916	22.078
ATOM	151	CA	ILE	A	15	-15.642	0.347	20.400
ATOM	152	C	ILE	A	15	-16.894	-0.328	19.887
ATOM	153	O	ILE	A	15	-17.115	-1.542	20.041
ATOM	154	CB	ILE	A	15	-14.382	-0.132	19.639
ATOM	155	CG1	ILE	A	15	-14.478	0.148	18.125
ATOM	156	CG2	ILE	A	15	-14.082	-1.623	19.880
ATOM	157	CD1	ILE	A	15	-14.237	1.603	17.796
ATOM	158	N	GLY	A	16	-17.843	0.435	19.308
ATOM	159	H	GLY	A	16	-17.720	1.426	19.260
ATOM	160	CA	GLY	A	16	-19.053	-0.143	18.745
ATOM	161	C	GLY	A	16	-19.897	-0.817	19.789
ATOM	162	O	GLY	A	16	-20.774	-1.668	19.516
ATOM	163	N	GLY	A	17	-19.712	-0.493	21.088
ATOM	164	H	GLY	A	17	-19.038	0.204	21.334
ATOM	165	CA	GLY	A	17	-20.464	-1.126	22.160
ATOM	166	C	GLY	A	17	-19.718	-2.335	22.653
ATOM	167	O	GLY	A	17	-20.147	-3.098	23.540

FIG. 11 A-2

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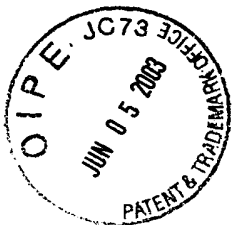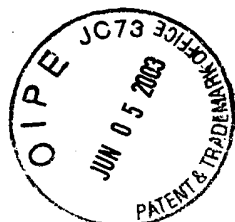Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
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Filed: 11/10/00   Attorney Docket No. 24737-1906C

ATOM	168	N	GLN	A	18	-18.507	-2.591	22.121
ATOM	169	H	GLN	A	18	-18.059	-1.900	21.554
ATOM	170	CA	GLN	A	18	-17.806	-3.830	22.326
ATOM	171	C	GLN	A	18	-16.552	-3.549	23.123
ATOM	172	O	GLN	A	18	-15.887	-2.508	22.945
ATOM	173	CB	GLN	A	18	-17.393	-4.294	20.928
ATOM	174	CG	GLN	A	18	-16.911	-5.734	20.788
ATOM	175	CD	GLN	A	18	-18.018	-6.728	20.613
ATOM	176	OE1	GLN	A	18	-19.131	-6.574	21.152
ATOM	177	NE2	GLN	A	18	-17.722	-7.773	19.857
ATOM	178	1HE2	GLN	A	18	-18.404	-8.484	19.689
ATOM	179	2HE2	GLN	A	18	-16.814	-7.860	19.448
ATOM	180	N	LEU	A	19	-16.133	-4.397	24.087
ATOM	181	H	LEU	A	19	-16.682	-5.202	24.312
ATOM	182	CA	LEU	A	19	-14.909	-4.178	24.808
ATOM	183	C	LEU	A	19	-13.799	-4.912	24.090
ATOM	184	O	LEU	A	19	-13.989	-6.018	23.558
ATOM	185	CB	LEU	A	19	-14.982	-4.714	26.254
ATOM	186	CG	LEU	A	19	-15.490	-3.778	27.374
ATOM	187	CD1	LEU	A	19	-16.392	-2.639	26.856
ATOM	188	CD2	LEU	A	19	-16.208	-4.516	28.465
ATOM	189	N	LYS	A	20	-12.603	-4.372	23.978
ATOM	190	H	LYS	A	20	-12.442	-3.448	24.324
ATOM	191	CA	LYS	A	20	-11.507	-5.082	23.365
ATOM	192	C	LYS	A	20	-10.266	-4.618	24.062
ATOM	193	O	LYS	A	20	-10.228	-3.611	24.816
ATOM	194	CB	LYS	A	20	-11.397	-4.798	21.875
ATOM	195	CG	LYS	A	20	-12.558	-5.356	21.100
ATOM	196	CD	LYS	A	20	-12.537	-4.988	19.615
ATOM	197	CE	LYS	A	20	-13.414	-5.958	18.827
ATOM	198	NZ	LYS	A	20	-12.681	-7.208	18.639
ATOM	199	1HZ	LYS	A	20	-13.247	-7.852	18.123
ATOM	200	3HZ	LYS	A	20	-12.458	-7.601	19.531
ATOM	201	2HZ	LYS	A	20	-11.837	-7.027	18.134
ATOM	202	N	GLU	A	21	-9.150	-5.357	23.893
ATOM	203	H	GLU	A	21	-9.185	-6.188	23.338
ATOM	204	CA	GLU	A	21	-7.890	-4.997	24.486
ATOM	205	C	GLU	A	21	-7.001	-4.462	23.390
ATOM	206	O	GLU	A	21	-6.970	-4.992	22.258
ATOM	207	CB	GLU	A	21	-7.268	-6.260	25.051
ATOM	208	CG	GLU	A	21	-5.835	-6.140	25.480
ATOM	209	CD	GLU	A	21	-5.405	-7.352	26.275
ATOM	210	OE1	GLU	A	21	-5.624	-7.343	27.508
ATOM	211	OE2	GLU	A	21	-4.852	-8.309	25.684
ATOM	212	N	ALA	A	22	-6.239	-3.369	23.595
ATOM	213	H	ALA	A	22	-6.223	-2.938	24.497
ATOM	214	CA	ALA	A	22	-5.419	-2.781	22.520
ATOM	215	C	ALA	A	22	-4.138	-2.255	23.114
ATOM	216	O	ALA	A	22	-3.985	-1.914	24.314
ATOM	217	CB	ALA	A	22	-6.134	-1.657	21.821
ATOM	218	N	LEU	A	23	-3.121	-2.091	22.240
ATOM	219	H	LEU	A	23	-3.279	-2.236	21.263
ATOM	220	CA	LEU	A	23	-1.797	-1.712	22.640
ATOM	221	C	LEU	A	23	-1.660	-0.230	22.443
ATOM	222	O	LEU	A	23	-2.020	0.349	21.402
ATOM	223	CB	LEU	A	23	-0.814	-2.486	21.732

FIG. II A-3

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ATOM	224	CG	LEU	A	23	0.705	-2.448	21.991
ATOM	225	CD1	LEU	A	23	1.088	-3.400	23.124
ATOM	226	CD2	LEU	A	23	1.462	-2.878	20.708
ATOM	227	N	LEU	A	24	-1.192	0.530	23.463
ATOM	228	H	LEU	A	24	-1.015	0.110	24.353
ATOM	229	CA	LEU	A	24	-0.935	1.952	23.305
ATOM	230	C	LEU	A	24	0.403	2.089	22.609
ATOM	231	O	LEU	A	24	1.471	1.717	23.130
ATOM	232	CB	LEU	A	24	-0.921	2.609	24.681
ATOM	233	CG	LEU	A	24	-2.220	2.492	25.477
ATOM	234	CD1	LEU	A	24	-2.063	3.291	26.772
ATOM	235	CD2	LEU	A	24	-3.419	3.000	24.691
ATOM	236	N	ASP	A	25	0.454	2.590	21.397
ATOM	237	H	ASP	A	25	-0.334	3.085	21.032
ATOM	238	CA	ASP	A	25	1.642	2.423	20.605
ATOM	239	C	ASP	A	25	2.130	3.750	20.059
ATOM	240	O	ASP	A	25	1.568	4.320	19.110
ATOM	241	CB	ASP	A	25	1.263	1.435	19.486
ATOM	242	CG	ASP	A	25	2.428	1.051	18.561
ATOM	243	OD1	ASP	A	25	3.546	1.540	18.729
ATOM	244	OD2	ASP	A	25	2.164	0.241	17.658
ATOM	245	N	THR	A	26	3.203	4.337	20.605
ATOM	246	H	THR	A	26	3.694	3.880	21.346
ATOM	247	CA	THR	A	26	3.691	5.652	20.144
ATOM	248	C	THR	A	26	4.397	5.583	18.778
ATOM	249	O	THR	A	26	4.642	6.587	18.079
ATOM	250	CB	THR	A	26	4.596	6.219	21.217
ATOM	251	OG1	THR	A	26	5.716	5.324	21.386
ATOM	252	HG1	THR	A	26	6.332	5.676	22.091
ATOM	253	CG2	THR	A	26	3.878	6.320	22.577
ATOM	254	N	GLY	A	27	4.757	4.377	18.298
ATOM	255	H	GLY	A	27	4.526	3.550	18.811
ATOM	256	CA	GLY	A	27	5.481	4.233	17.040
ATOM	257	C	GLY	A	27	4.520	4.190	15.886
ATOM	258	O	GLY	A	27	4.908	4.242	14.696
ATOM	259	N	ALA	A	28	3.197	4.084	16.117
ATOM	260	H	ALA	A	28	2.856	4.091	17.057
ATOM	261	CA	ALA	A	28	2.213	3.955	15.018
ATOM	262	C	ALA	A	28	1.598	5.299	14.750
ATOM	263	O	ALA	A	28	1.062	5.982	15.650
ATOM	264	CB	ALA	A	28	1.117	2.980	15.390
ATOM	265	N	ASP	A	29	1.503	5.744	13.490
ATOM	266	H	ASP	A	29	1.912	5.216	12.746
ATOM	267	CA	ASP	A	29	0.810	6.984	13.213
ATOM	268	C	ASP	A	29	-0.666	6.724	13.327
ATOM	269	O	ASP	A	29	-1.488	7.637	13.568
ATOM	270	CB	ASP	A	29	1.009	7.433	11.775
ATOM	271	CG	ASP	A	29	2.439	7.882	11.412
ATOM	272	OD1	ASP	A	29	3.360	7.856	12.269
ATOM	273	OD2	ASP	A	29	2.606	8.253	10.252
ATOM	274	N	ASP	A	30	-1.143	5.517	12.990
ATOM	275	H	ASP	A	30	-0.508	4.769	12.800
ATOM	276	CA	ASP	A	30	-2.579	5.245	12.887
ATOM	277	C	ASP	A	30	-3.057	4.208	13.867
ATOM	278	O	ASP	A	30	-2.284	3.483	14.546
ATOM	279	CB	ASP	A	30	-2.896	4.758	11.456

FIG. 11 A-4

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ATOM	280	CG	ASP	A	30	-2.495	5.768	10.425
ATOM	281	OD1	ASP	A	30	-3.067	6.871	10.423
ATOM	282	OD2	ASP	A	30	-1.596	5.494	9.618
ATOM	283	N	THR	A	31	-4.393	4.076	14.002
ATOM	284	H	THR	A	31	-5.004	4.700	13.515
ATOM	285	CA	THR	A	31	-5.059	3.062	14.829
ATOM	286	C	THR	A	31	-5.565	1.967	13.913
ATOM	287	O	THR	A	31	-6.223	2.169	12.870
ATOM	288	CB	THR	A	31	-6.212	3.725	15.566
ATOM	289	OG1	THR	A	31	-5.668	4.667	16.474
ATOM	290	HG1	THR	A	31	-6.403	5.122	16.976
ATOM	291	CG2	THR	A	31	-7.044	2.702	16.389
ATOM	292	N	VAL	A	32	-5.187	0.713	14.235
ATOM	293	H	VAL	A	32	-4.649	0.555	15.063
ATOM	294	CA	VAL	A	32	-5.517	-0.462	13.437
ATOM	295	C	VAL	A	32	-6.092	-1.506	14.365
ATOM	296	O	VAL	A	32	-5.502	-1.957	15.365
ATOM	297	CB	VAL	A	32	-4.260	-1.064	12.757
ATOM	298	CG1	VAL	A	32	-4.667	-2.136	11.735
ATOM	299	CG2	VAL	A	32	-3.422	0.017	12.032
ATOM	300	N	LEU	A	33	-7.352	-1.923	14.119
ATOM	301	H	LEU	A	33	-7.867	-1.523	13.361
ATOM	302	CA	LEU	A	33	-7.982	-2.940	14.929
ATOM	303	C	LEU	A	33	-8.174	-4.203	14.107
ATOM	304	O	LEU	A	33	-8.268	-4.247	12.853
ATOM	305	CB	LEU	A	33	-9.336	-2.477	15.408
ATOM	306	CG	LEU	A	33	-9.292	-1.149	16.127
ATOM	307	CD1	LEU	A	33	-10.710	-0.747	16.485
ATOM	308	CD2	LEU	A	33	-8.348	-1.139	17.347
ATOM	309	N	GLU	A	34	-8.296	-5.319	14.782
ATOM	310	H	GLU	A	34	-8.244	-5.302	15.780
ATOM	311	CA	GLU	A	34	-8.503	-6.551	14.086
ATOM	312	C	GLU	A	34	-9.909	-6.549	13.510
ATOM	313	O	GLU	A	34	-10.808	-5.717	13.795
ATOM	314	CB	GLU	A	34	-8.265	-7.750	15.010
ATOM	315	CG	GLU	A	34	-9.259	-7.791	16.165
ATOM	316	CD	GLU	A	34	-8.763	-8.552	17.404
ATOM	317	OE1	GLU	A	34	-7.670	-9.193	17.368
ATOM	318	OE2	GLU	A	34	-9.482	-8.497	18.407
ATOM	319	N	GLU	A	35	-10.152	-7.480	12.568
ATOM	320	H	GLU	A	35	-9.485	-8.208	12.407
ATOM	321	CA	GLU	A	35	-11.352	-7.466	11.773
ATOM	322	C	GLU	A	35	-12.631	-7.520	12.571
ATOM	323	O	GLU	A	35	-12.814	-8.294	13.528
ATOM	324	CB	GLU	A	35	-11.237	-8.536	10.707
ATOM	325	CG	GLU	A	35	-9.945	-8.280	9.907
ATOM	326	CD	GLU	A	35	-9.872	-8.872	8.486
ATOM	327	OE1	GLU	A	35	-10.612	-8.401	7.603
ATOM	328	OE2	GLU	A	35	-9.024	-9.776	8.261
ATOM	329	N	MET	A	36	-13.580	-6.598	12.278
ATOM	330	H	MET	A	36	-13.439	-5.967	11.515
ATOM	331	CA	MET	A	36	-14.819	-6.495	13.052
ATOM	332	C	MET	A	36	-15.826	-5.635	12.271
ATOM	333	O	MET	A	36	-15.514	-4.828	11.371
ATOM	334	CB	MET	A	36	-14.593	-5.845	14.428
ATOM	335	CG	MET	A	36	-14.279	-4.353	14.417

FIG. 11A-5
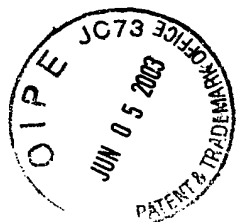
Heller Ehrman White & McAuliffe, LLP
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Title: Use of Computationally Derived Protein Structures of Genetic
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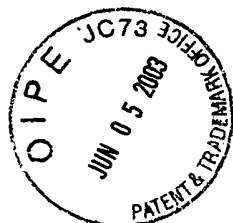Serial No.: 09/709,905   Applicants: Ramnarayan *et al.*
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ATOM	336	SD	MET	A	36	-14.251	-3.718	16.099
ATOM	337	CE	MET	A	36	-12.487	-3.846	16.409
ATOM	338	N	SER	A	37	-17.130	-5.776	12.590
ATOM	339	H	SER	A	37	-17.399	-6.431	13.296
ATOM	340	CA	SER	A	37	-18.155	-5.005	11.940
ATOM	341	C	SER	A	37	-18.286	-3.693	12.657
ATOM	342	O	SER	A	37	-18.593	-3.624	13.865
ATOM	343	CB	SER	A	37	-19.506	-5.688	12.032
ATOM	344	OG	SER	A	37	-19.455	-7.054	11.716
ATOM	345	HG	SER	A	37	-20.367	-7.457	11.791
ATOM	346	N	LEU	A	38	-18.185	-2.569	11.933
ATOM	347	H	LEU	A	38	-17.956	-2.625	10.952
ATOM	348	CA	LEU	A	38	-18.557	-1.247	12.465
ATOM	349	C	LEU	A	38	-19.630	-0.605	11.572
ATOM	350	O	LEU	A	38	-19.706	-0.939	10.391
ATOM	351	CB	LEU	A	38	-17.315	-0.346	12.588
ATOM	352	CG	LEU	A	38	-16.246	-0.818	13.596
ATOM	353	CD1	LEU	A	38	-14.998	0.073	13.489
ATOM	354	CD2	LEU	A	38	-16.756	-0.787	15.046
ATOM	355	N	PRO	A	39	-20.455	0.321	12.108
ATOM	356	CA	PRO	A	39	-21.460	1.053	11.339
ATOM	357	C	PRO	A	39	-20.824	2.176	10.502
ATOM	358	O	PRO	A	39	-19.654	2.519	10.685
ATOM	359	CB	PRO	A	39	-22.430	1.607	12.389
ATOM	360	CG	PRO	A	39	-21.531	1.845	13.600
ATOM	361	CD	PRO	A	39	-20.539	0.686	13.517
ATOM	362	N	GLY	A	40	-21.620	2.749	9.586
ATOM	363	H	GLY	A	40	-22.569	2.417	9.493
ATOM	364	CA	GLY	A	40	-21.203	3.811	8.678
ATOM	365	C	GLY	A	40	-20.836	3.262	7.298
ATOM	366	O	GLY	A	40	-21.405	2.268	6.845
ATOM	367	N	LYS	A	41	-19.895	3.945	6.631
ATOM	368	H	LYS	A	41	-19.496	4.761	7.071
ATOM	369	CA	LYS	A	41	-19.323	3.558	5.343
ATOM	370	C	LYS	A	41	-17.798	3.757	5.371
ATOM	371	O	LYS	A	41	-17.263	4.462	6.229
ATOM	372	CB	LYS	A	41	-20.025	4.352	4.224
ATOM	373	CG	LYS	A	41	-19.703	3.839	2.810
ATOM	374	CD	LYS	A	41	-20.610	4.486	1.757
ATOM	375	CE	LYS	A	41	-20.240	3.964	0.366
ATOM	376	NZ	LYS	A	41	-21.097	4.552	-0.678
ATOM	377	1HZ	LYS	A	41	-20.824	4.189	-1.580
ATOM	378	3HZ	LYS	A	41	-20.993	5.556	-0.673
ATOM	379	2HZ	LYS	A	41	-22.061	4.311	-0.498
ATOM	380	N	TRP	A	42	-17.104	3.091	4.439
ATOM	381	H	TRP	A	42	-17.620	2.548	3.762
ATOM	382	CA	TRP	A	42	-15.654	2.932	4.423
ATOM	383	C	TRP	A	42	-15.105	2.852	2.994
ATOM	384	O	TRP	A	42	-15.845	2.702	2.021
ATOM	385	CB	TRP	A	42	-15.279	1.675	5.236
ATOM	386	CG	TRP	A	42	-16.214	0.514	5.094
ATOM	387	CD1	TRP	A	42	-16.230	-0.402	4.101
ATOM	388	CD2	TRP	A	42	-17.355	0.203	5.942
ATOM	389	NE1	TRP	A	42	-17.297	-1.260	4.281
ATOM	390	HE1	TRP	A	42	-17.504	-2.015	3.644
ATOM	391	CE2	TRP	A	42	-18.045	-0.914	5.389

FIG. 11A-6

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| ATOM	392	CE3	TRP	A	42	-17.896	0.792	7.103
ATOM	393	CZ2	TRP	A	42	-19.224	-1.421	5.959
ATOM	394	CZ3	TRP	A	42	-19.077	0.298	7.675
ATOM	395	CH2	TRP	A	42	-19.741	-0.806	7.112
ATOM	396	N	LYS	A	43	-13.771	2.932	2.911
ATOM	397	H	LYS	A	43	-13.260	3.058	3.773
ATOM	398	CA	LYS	A	43	-12.951	2.802	1.713
ATOM	399	C	LYS	A	43	-11.773	1.859	2.012
ATOM	400	O	LYS	A	43	-11.359	1.760	3.166
ATOM	401	CB	LYS	A	43	-12.451	4.193	1.270
ATOM	402	CG	LYS	A	43	-11.724	4.979	2.383
ATOM	403	CD	LYS	A	43	-11.060	6.267	1.873
ATOM	404	CE	LYS	A	43	-9.784	6.001	1.065
ATOM	405	NZ	LYS	A	43	-8.700	5.458	1.903
ATOM	406	1HZ	LYS	A	43	-7.876	5.315	1.338
ATOM	407	3HZ	LYS	A	43	-8.993	4.576	2.300
ATOM	408	2HZ	LYS	A	43	-8.493	6.108	2.647
ATOM	409	N	PRO	A	44	-11.177	1.197	1.004
ATOM	410	CA	PRO	A	44	-9.947	0.435	1.187
ATOM	411	C	PRO	A	44	-8.760	1.392	1.379
ATOM	412	O	PRO	A	44	-8.711	2.434	0.720
ATOM	413	CB	PRO	A	44	-9.808	-0.393	-0.095
ATOM	414	CG	PRO	A	44	-10.501	0.458	-1.159
ATOM	415	CD	PRO	A	44	-11.630	1.132	-0.380
ATOM	416	N	LYS	A	45	-7.790	1.030	2.240
ATOM	417	H	LYS	A	45	-7.912	0.227	2.824
ATOM	418	CA	LYS	A	45	-6.547	1.747	2.314
ATOM	419	C	LYS	A	45	-5.493	0.683	2.507
ATOM	420	O	LYS	A	45	-5.780	-0.470	2.869
ATOM	421	CB	LYS	A	45	-6.594	2.699	3.524
ATOM	422	CG	LYS	A	45	-5.463	3.744	3.609
ATOM	423	CD	LYS	A	45	-5.340	4.289	5.052
ATOM	424	CE	LYS	A	45	-4.262	5.383	5.204
ATOM	425	NZ	LYS	A	45	-2.907	4.911	4.916
ATOM	426	1HZ	LYS	A	45	-2.260	5.664	5.032
ATOM	427	3HZ	LYS	A	45	-2.864	4.577	3.975
ATOM	428	2HZ	LYS	A	45	-2.672	4.169	5.544
ATOM	429	N	MET	A	46	-4.224	0.949	2.193
ATOM	430	H	MET	A	46	-3.998	1.805	1.728
ATOM	431	CA	MET	A	46	-3.157	0.027	2.509
ATOM	432	C	MET	A	46	-2.417	0.701	3.627
ATOM	433	O	MET	A	46	-2.259	1.937	3.634
ATOM	434	CB	MET	A	46	-2.166	-0.088	1.379
ATOM	435	CG	MET	A	46	-2.782	-0.366	0.053
ATOM	436	SD	MET	A	46	-3.076	-2.108	-0.118
ATOM	437	CE	MET	A	46	-1.417	-2.652	-0.186
ATOM	438	N	ILE	A	47	-1.827	-0.016	4.586
ATOM	439	H	ILE	A	47	-2.010	-0.997	4.655
ATOM	440	CA	ILE	A	47	-0.922	0.586	5.539
ATOM	441	C	ILE	A	47	0.233	-0.372	5.654
ATOM	442	O	ILE	A	47	0.135	-1.584	5.356
ATOM	443	CB	ILE	A	47	-1.550	0.836	6.923
ATOM	444	CG1	ILE	A	47	-2.459	-0.301	7.354
ATOM	445	CG2	ILE	A	47	-2.248	2.164	6.995
ATOM	446	CD1	ILE	A	47	-1.724	-1.336	8.111
ATOM	447	N	GLY	A	48	1.420	0.089	6.043

FIG. 11A-7
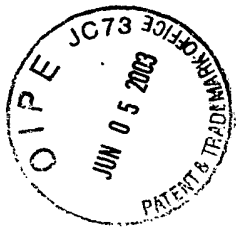
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| ATOM	448	H	GLY	A	48	1.509	1.040	6.339
ATOM	449	CA	GLY	A	48	2.584	-0.753	6.048
ATOM	450	C	GLY	A	48	3.280	-0.657	7.376
ATOM	451	O	GLY	A	48	3.050	0.190	8.265
ATOM	452	N	GLY	A	49	4.197	-1.617	7.603
ATOM	453	H	GLY	A	49	4.375	-2.308	6.902
ATOM	454	CA	GLY	A	49	4.936	-1.684	8.828
ATOM	455	C	GLY	A	49	6.105	-2.589	8.533
ATOM	456	O	GLY	A	49	6.482	-2.807	7.370
ATOM	457	N	ILE	A	50	6.761	-3.173	9.552
ATOM	458	H	ILE	A	50	6.552	-2.908	10.493
ATOM	459	CA	ILE	A	50	7.772	-4.184	9.344
ATOM	460	C	ILE	A	50	7.148	-5.317	8.566
ATOM	461	O	ILE	A	50	5.981	-5.734	8.772
ATOM	462	CB	ILE	A	50	8.258	-4.686	10.722
ATOM	463	CG1	ILE	A	50	9.257	-3.714	11.382
ATOM	464	CG2	ILE	A	50	8.813	-6.134	10.693
ATOM	465	CD1	ILE	A	50	10.580	-3.498	10.628
ATOM	466	N	GLY	A	51	7.847	-5.891	7.596
ATOM	467	H	GLY	A	51	8.772	-5.569	7.395
ATOM	468	CA	GLY	A	51	7.265	-6.966	6.850
ATOM	469	C	GLY	A	51	6.519	-6.559	5.591
ATOM	470	O	GLY	A	51	6.430	-7.318	4.634
ATOM	471	N	GLY	A	52	5.886	-5.375	5.517
ATOM	472	H	GLY	A	52	5.990	-4.710	6.257
ATOM	473	CA	GLY	A	52	5.108	-5.227	4.320
ATOM	474	C	GLY	A	52	3.832	-4.415	4.516
ATOM	475	O	GLY	A	52	3.654	-3.624	5.467
ATOM	476	N	PHE	A	53	2.886	-4.518	3.559
ATOM	477	H	PHE	A	53	3.013	-5.161	2.804
ATOM	478	CA	PHE	A	53	1.653	-3.720	3.566
ATOM	479	C	PHE	A	53	0.494	-4.651	3.783
ATOM	480	O	PHE	A	53	0.448	-5.816	3.336
ATOM	481	CB	PHE	A	53	1.424	-3.022	2.221
ATOM	482	CG	PHE	A	53	2.363	-1.896	2.008
ATOM	483	CD1	PHE	A	53	3.615	-2.135	1.447
ATOM	484	CD2	PHE	A	53	2.011	-0.608	2.414
ATOM	485	CE1	PHE	A	53	4.514	-1.087	1.275
ATOM	486	CE2	PHE	A	53	2.925	0.446	2.237
ATOM	487	CZ	PHE	A	53	4.172	0.202	1.668
ATOM	488	N	ILE	A	54	-0.554	-4.173	4.439
ATOM	489	H	ILE	A	54	-0.491	-3.285	4.895
ATOM	490	CA	ILE	A	54	-1.789	-4.911	4.509
ATOM	491	C	ILE	A	54	-2.903	-3.995	4.033
ATOM	492	O	ILE	A	54	-2.751	-2.770	3.855
ATOM	493	CB	ILE	A	54	-2.034	-5.535	5.904
ATOM	494	CG1	ILE	A	54	-2.343	-4.481	6.988
ATOM	495	CG2	ILE	A	54	-0.799	-6.318	6.314
ATOM	496	CD1	ILE	A	54	-3.010	-5.089	8.246
ATOM	497	N	LYS	A	55	-4.029	-4.577	3.560
ATOM	498	H	LYS	A	55	-4.084	-5.574	3.501
ATOM	499	CA	LYS	A	55	-5.177	-3.798	3.129
ATOM	500	C	LYS	A	55	-6.115	-3.726	4.300
ATOM	501	O	LYS	A	55	-6.422	-4.707	5.023
ATOM	502	CB	LYS	A	55	-5.928	-4.461	1.938
ATOM	503	CG	LYS	A	55	-6.853	-3.547	1.106

FIG. 11 A-8
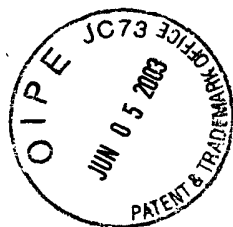
Heller Ehrman White & McAuliffe, LLP
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Title: Use of Computationally Derived Protein Structures of Genetic
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ATOM	504	CD	LYS	A	55	-8.267	-3.332	1.714
ATOM	505	CE	LYS	A	55	-9.303	-4.392	1.301
ATOM	506	NZ	LYS	A	55	-10.521	-4.453	2.192
ATOM	507	1HZ	LYS	A	55	-11.142	-5.162	1.859
ATOM	508	3HZ	LYS	A	55	-10.987	-3.569	2.180
ATOM	509	2HZ	LYS	A	55	-10.240	-4.669	3.127
ATOM	510	N	VAL	A	56	-6.599	-2.509	4.619
ATOM	511	H	VAL	A	56	-6.337	-1.713	4.073
ATOM	512	CA	VAL	A	56	-7.494	-2.311	5.735
ATOM	513	C	VAL	A	56	-8.711	-1.584	5.236
ATOM	514	O	VAL	A	56	-8.767	-1.029	4.114
ATOM	515	CB	VAL	A	56	-6.759	-1.475	6.812
ATOM	516	CG1	VAL	A	56	-5.569	-2.209	7.385
ATOM	517	CG2	VAL	A	56	-6.287	-0.108	6.268
ATOM	518	N	ARG	A	57	-9.784	-1.539	6.005
ATOM	519	H	ARG	A	57	-9.835	-2.117	6.819
ATOM	520	CA	ARG	A	57	-10.855	-0.648	5.638
ATOM	521	C	ARG	A	57	-10.738	0.534	6.554
ATOM	522	O	ARG	A	57	-10.558	0.449	7.789
ATOM	523	CB	ARG	A	57	-12.219	-1.271	5.835
ATOM	524	CG	ARG	A	57	-12.480	-2.452	4.952
ATOM	525	CD	ARG	A	57	-13.834	-3.051	5.195
ATOM	526	NE	ARG	A	57	-14.122	-4.137	4.270
ATOM	527	HE	ARG	A	57	-13.442	-4.347	3.568
ATOM	528	CZ	ARG	A	57	-15.243	-4.851	4.324
ATOM	529	NH1	ARG	A	57	-16.175	-4.624	5.243
ATOM	530	2HH1	ARG	A	57	-16.044	-3.899	5.920
ATOM	531	1HH1	ARG	A	57	-17.008	-5.178	5.258
ATOM	532	NH2	ARG	A	57	-15.433	-5.822	3.434
ATOM	533	1HH2	ARG	A	57	-16.270	-6.368	3.461
ATOM	534	2HH2	ARG	A	57	-14.738	-6.006	2.738
ATOM	535	N	GLN	A	58	-10.881	1.741	6.036
ATOM	536	H	GLN	A	58	-11.030	1.844	5.053
ATOM	537	CA	GLN	A	58	-10.830	2.922	6.839
ATOM	538	C	GLN	A	58	-12.231	3.342	7.205
ATOM	539	O	GLN	A	58	-13.106	3.608	6.359
ATOM	540	CB	GLN	A	58	-10.208	4.038	6.030
ATOM	541	CG	GLN	A	58	-10.055	5.293	6.817
ATOM	542	CD	GLN	A	58	-9.632	6.411	5.927
ATOM	543	OE1	GLN	A	58	-10.379	7.334	5.662
ATOM	544	NE2	GLN	A	58	-8.412	6.303	5.437
ATOM	545	1HE2	GLN	A	58	-8.047	7.009	4.830
ATOM	546	2HE2	GLN	A	58	-7.843	5.514	5.668
ATOM	547	N	TYR	A	59	-12.527	3.516	8.509
ATOM	548	H	TYR	A	59	-11.877	3.219	9.209
ATOM	549	CA	TYR	A	59	-13.769	4.125	8.933
ATOM	550	C	TYR	A	59	-13.411	5.452	9.565
ATOM	551	O	TYR	A	59	-12.416	5.592	10.310
ATOM	552	CB	TYR	A	59	-14.517	3.252	9.957
ATOM	553	CG	TYR	A	59	-14.287	1.770	9.723
ATOM	554	CD1	TYR	A	59	-13.007	1.269	9.457
ATOM	555	CD2	TYR	A	59	-15.346	0.865	9.766
ATOM	556	CE1	TYR	A	59	-12.797	-0.092	9.240
ATOM	557	CE2	TYR	A	59	-15.148	-0.494	9.551
ATOM	558	CZ	TYR	A	59	-13.873	-0.972	9.287
ATOM	559	OH	TYR	A	59	-13.721	-2.311	9.079

FIG. 11 A-9
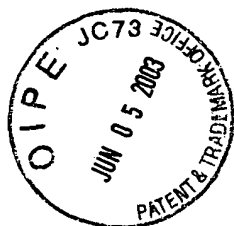
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Title: Use of Computationally Derived Protein Structures of Genetic
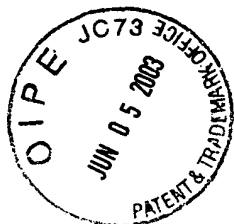Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
Serial No.: 09/709,905   Applicants: Ramnarayan *et al.*
Filed: 11/10/00   Attorney Docket No. 24737-1906C

ATOM	560	HH	TYR	A	59	-14.606	-2.771	9.154
ATOM	561	N	ASP	A	60	-14.151	6.542	9.300
ATOM	562	H	ASP	A	60	-14.954	6.464	8.709
ATOM	563	CA	ASP	A	60	-13.822	7.836	9.846
ATOM	564	C	ASP	A	60	-14.782	8.226	10.947
ATOM	565	O	ASP	A	60	-15.941	7.765	11.053
ATOM	566	CB	ASP	A	60	-13.861	8.942	8.769
ATOM	567	CG	ASP	A	60	-12.735	8.830	7.725
ATOM	568	OD1	ASP	A	60	-11.545	8.874	8.075
ATOM	569	OD2	ASP	A	60	-13.060	8.702	6.544
ATOM	570	N	GLN	A	61	-14.339	9.154	11.833
ATOM	571	H	GLN	A	61	-13.385	9.451	11.804
ATOM	572	CA	GLN	A	61	-15.151	9.804	12.885
ATOM	573	C	GLN	A	61	-15.839	8.803	13.802
ATOM	574	O	GLN	A	61	-17.008	8.893	14.229
ATOM	575	CB	GLN	A	61	-16.097	10.908	12.338
ATOM	576	CG	GLN	A	61	-16.239	12.133	13.262
ATOM	577	CD	GLN	A	61	-16.910	13.366	12.629
ATOM	578	OE1	GLN	A	61	-16.509	13.854	11.586
ATOM	579	NE2	GLN	A	61	-17.937	13.887	13.292
ATOM	580	1HE2	GLN	A	61	-18.416	14.689	12.934
ATOM	581	2HE2	GLN	A	61	-18.239	13.482	14.155
ATOM	582	N	ILE	A	62	-15.060	7.760	14.175
ATOM	583	H	ILE	A	62	-14.111	7.714	13.862
ATOM	584	CA	ILE	A	62	-15.557	6.705	15.015
ATOM	585	C	ILE	A	62	-15.251	7.057	16.447
ATOM	586	O	ILE	A	62	-14.198	7.613	16.837
ATOM	587	CB	ILE	A	62	-14.829	5.397	14.653
ATOM	588	CG1	ILE	A	62	-15.253	4.966	13.258
ATOM	589	CG2	ILE	A	62	-15.106	4.271	15.675
ATOM	590	CD1	ILE	A	62	-16.779	4.788	13.116
ATOM	591	N	LEU	A	63	-16.242	6.807	17.320
ATOM	592	H	LEU	A	63	-17.089	6.383	17.000
ATOM	593	CA	LEU	A	63	-16.127	7.131	18.719
ATOM	594	C	LEU	A	63	-15.518	5.942	19.425
ATOM	595	O	LEU	A	63	-15.869	4.753	19.269
ATOM	596	CB	LEU	A	63	-17.512	7.428	19.282
ATOM	597	CG	LEU	A	63	-17.660	7.598	20.813
ATOM	598	CD1	LEU	A	63	-16.711	8.632	21.404
ATOM	599	CD2	LEU	A	63	-19.089	7.963	21.201
ATOM	600	N	ILE	A	64	-14.511	6.211	20.219
ATOM	601	H	ILE	A	64	-14.185	7.153	20.305
ATOM	602	CA	ILE	A	64	-13.862	5.178	20.972
ATOM	603	C	ILE	A	64	-13.529	5.744	22.325
ATOM	604	O	ILE	A	64	-13.396	6.959	22.602
ATOM	605	CB	ILE	A	64	-12.618	4.716	20.231
ATOM	606	CG1	ILE	A	64	-11.925	3.573	20.949
ATOM	607	CG2	ILE	A	64	-11.690	5.865	19.950
ATOM	608	CD1	ILE	A	64	-10.905	2.888	20.062
ATOM	609	N	GLU	A	65	-13.396	4.815	23.294
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ATOM	611	CA	GLU	A	65	-13.186	5.174	24.670
ATOM	612	C	GLU	A	65	-12.024	4.360	25.165
ATOM	613	O	GLU	A	65	-11.943	3.112	25.056
ATOM	614	CB	GLU	A	65	-14.459	4.823	25.405
ATOM	615	CG	GLU	A	65	-14.739	5.610	26.646

FIG. 11A-10

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Title: Use of Computationally Derived Protein Structures of Genetic
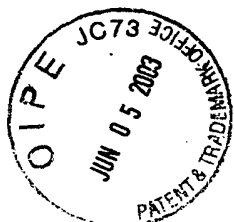Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
Serial No.: 09/709,905   Applicants: Ramnarayan et al.
Filed: 11/10/00   Attorney Docket No. 24737-1906C

|								
ATOM	616	CD	GLU	A	65	-16.131	5.353	27.115
ATOM	617	OE1	GLU	A	65	-17.090	5.785	26.413
ATOM	618	OE2	GLU	A	65	-16.269	4.708	28.163
ATOM	619	N	ILE	A	66	-10.971	5.008	25.610
ATOM	620	H	ILE	A	66	-11.009	6.002	25.717
ATOM	621	CA	ILE	A	66	-9.762	4.317	25.947
ATOM	622	C	ILE	A	66	-9.571	4.586	27.413
ATOM	623	O	ILE	A	66	-9.422	5.732	27.880
ATOM	624	CB	ILE	A	66	-8.600	4.907	25.126
ATOM	625	CG1	ILE	A	66	-8.838	4.669	23.633
ATOM	626	CG2	ILE	A	66	-7.231	4.326	25.554
ATOM	627	CD1	ILE	A	66	-8.951	5.982	22.856
ATOM	628	N	CYS	A	67	-9.776	3.567	28.261
ATOM	629	H	CYS	A	67	-9.989	2.659	27.902
ATOM	630	CA	CYS	A	67	-9.698	3.740	29.687
ATOM	631	C	CYS	A	67	-10.673	4.871	30.088
ATOM	632	O	CYS	A	67	-10.393	5.716	30.958
ATOM	633	CB	CYS	A	67	-8.251	4.003	30.156
ATOM	634	SG	CYS	A	67	-7.170	2.529	30.217
ATOM	635	N	GLY	A	68	-11.877	4.947	29.499
ATOM	636	H	GLY	A	68	-12.125	4.286	28.791
ATOM	637	CA	GLY	A	68	-12.788	5.984	29.903
ATOM	638	C	GLY	A	68	-12.581	7.322	29.241
ATOM	639	O	GLY	A	68	-13.404	8.253	29.376
ATOM	640	N	HIS	A	69	-11.504	7.545	28.471
ATOM	641	H	HIS	A	69	-10.817	6.827	28.360
ATOM	642	CA	HIS	A	69	-11.305	8.800	27.793
ATOM	643	C	HIS	A	69	-11.838	8.679	26.399
ATOM	644	O	HIS	A	69	-11.516	7.742	25.630
ATOM	645	CB	HIS	A	69	-9.831	9.128	27.724
ATOM	646	CG	HIS	A	69	-9.276	9.286	29.081
ATOM	647	ND1	HIS	A	69	-9.317	10.484	29.778
ATOM	648	HD1	HIS	A	69	-9.688	11.347	29.436
ATOM	649	CD2	HIS	A	69	-8.723	8.352	29.912
ATOM	650	CE1	HIS	A	69	-8.783	10.254	30.947
ATOM	651	NE2	HIS	A	69	-8.405	8.990	31.091
ATOM	652	N	LYS	A	70	-12.768	9.561	25.973
ATOM	653	H	LYS	A	70	-13.084	10.284	26.588
ATOM	654	CA	LYS	A	70	-13.325	9.492	24.646
ATOM	655	C	LYS	A	70	-12.346	10.074	23.653
ATOM	656	O	LYS	A	70	-11.587	11.055	23.864
ATOM	657	CB	LYS	A	70	-14.645	10.285	24.536
ATOM	658	CG	LYS	A	70	-15.837	9.703	25.330
ATOM	659	CD	LYS	A	70	-17.105	10.593	25.286
ATOM	660	CE	LYS	A	70	-18.293	10.011	26.092
ATOM	661	NZ	LYS	A	70	-18.802	8.702	25.608
ATOM	662	1HZ	LYS	A	70	-19.563	8.406	26.185
ATOM	663	3HZ	LYS	A	70	-18.069	8.023	25.650
ATOM	664	2HZ	LYS	A	70	-19.116	8.795	24.663
ATOM	665	N	ALA	A	71	-12.323	9.485	22.446
ATOM	666	H	ALA	A	71	-12.813	8.625	22.305
ATOM	667	CA	ALA	A	71	-11.616	10.044	21.333
ATOM	668	C	ALA	A	71	-12.529	9.795	20.171
ATOM	669	O	ALA	A	71	-13.351	8.850	20.146
ATOM	670	CB	ALA	A	71	-10.292	9.358	21.143
ATOM	671	N	ILE	A	72	-12.559	10.685	19.149

FIG. IIA-II

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Filed: 11/10/00   Attorney Docket No. 24737-1906C

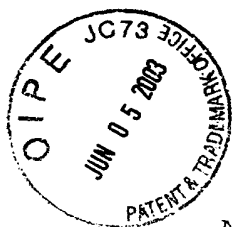|								
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ATOM	673	CA	ILE	A	72	-13.376	10.474	17.963
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ATOM	675	O	ILE	A	72	-11.858	11.720	16.550
ATOM	676	CB	ILE	A	72	-14.541	11.464	17.882
ATOM	677	CG1	ILE	A	72	-15.306	11.455	19.196
ATOM	678	CG2	ILE	A	72	-15.429	11.203	16.651
ATOM	679	CD1	ILE	A	72	-16.446	12.415	19.176
ATOM	680	N	GLY	A	73	-12.252	9.633	15.958
ATOM	681	H	GLY	A	73	-12.778	8.789	16.067
ATOM	682	CA	GLY	A	73	-11.253	9.755	14.938
ATOM	683	C	GLY	A	73	-11.283	8.554	14.034
ATOM	684	O	GLY	A	73	-12.211	7.706	14.006
ATOM	685	N	THR	A	74	-10.247	8.428	13.182
ATOM	686	H	THR	A	74	-9.471	9.055	13.250
ATOM	687	CA	THR	A	74	-10.201	7.416	12.158
ATOM	688	C	THR	A	74	-9.674	6.134	12.760
ATOM	689	O	THR	A	74	-8.670	6.034	13.497
ATOM	690	CB	THR	A	74	-9.298	7.895	11.048
ATOM	691	OG1	THR	A	74	-9.910	9.019	10.441
ATOM	692	HG1	THR	A	74	-9.335	9.362	9.698
ATOM	693	CG2	THR	A	74	-9.088	6.823	9.946
ATOM	694	N	VAL	A	75	-10.318	5.027	12.327
ATOM	695	H	VAL	A	75	-11.066	5.114	11.669
ATOM	696	CA	VAL	A	75	-9.968	3.717	12.778
ATOM	697	C	VAL	A	75	-9.906	2.843	11.551
ATOM	698	O	VAL	A	75	-10.803	2.807	10.681
ATOM	699	CB	VAL	A	75	-11.044	3.250	13.737
ATOM	700	CG1	VAL	A	75	-11.021	1.721	13.943
ATOM	701	CG2	VAL	A	75	-10.915	4.019	15.034
ATOM	702	N	LEU	A	76	-8.768	2.139	11.366
ATOM	703	H	LEU	A	76	-8.002	2.260	11.998
ATOM	704	CA	LEU	A	76	-8.566	1.183	10.276
ATOM	705	C	LEU	A	76	-8.848	-0.211	10.808
ATOM	706	O	LEU	A	76	-8.514	-0.582	11.958
ATOM	707	CB	LEU	A	76	-7.103	1.270	9.798
ATOM	708	CG	LEU	A	76	-6.608	2.684	9.443
ATOM	709	CD1	LEU	A	76	-5.151	2.645	9.087
ATOM	710	CD2	LEU	A	76	-7.396	3.302	8.296
ATOM	711	N	VAL	A	77	-9.569	-1.062	10.042
ATOM	712	H	VAL	A	77	-9.894	-0.766	9.144
ATOM	713	CA	VAL	A	77	-9.899	-2.428	10.485
ATOM	714	C	VAL	A	77	-9.298	-3.412	9.482
ATOM	715	O	VAL	A	77	-9.450	-3.300	8.253
ATOM	716	CB	VAL	A	77	-11.436	-2.592	10.506
ATOM	717	CG1	VAL	A	77	-11.830	-4.021	10.682
ATOM	718	CG2	VAL	A	77	-12.072	-1.765	11.634
ATOM	719	N	GLY	A	78	-8.560	-4.402	9.928
ATOM	720	H	GLY	A	78	-8.445	-4.530	10.913
ATOM	721	CA	GLY	A	78	-7.930	-5.285	8.987
ATOM	722	C	GLY	A	78	-7.228	-6.380	9.732
ATOM	723	O	GLY	A	78	-7.292	-6.524	10.970
ATOM	724	N	PRO	A	79	-6.512	-7.271	9.003
ATOM	725	CA	PRO	A	79	-5.880	-8.467	9.602
ATOM	726	C	PRO	A	79	-4.599	-8.107	10.340
ATOM	727	O	PRO	A	79	-3.449	-8.489	10.032

FIG. 11 A-12
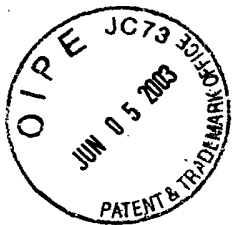
Heller Ehrman White & McAuliffe, LLP
Sheet 14 of 33
Title: Use of Computationally Derived Protein Structures of Genetic
Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
Serial No.: 09/709,905   Applicants: Ramnarayan *et al.*
Filed: 11/10/00   Attorney Docket No. 24737-1906C

ATOM	728	CB	PRO	A	79	-5.613	-9.379	8.400
ATOM	729	CG	PRO	A	79	-5.529	-8.416	7.210
ATOM	730	CD	PRO	A	79	-6.415	-7.225	7.537
ATOM	731	N	THR	A	80	-4.759	-7.304	11.408
ATOM	732	H	THR	A	80	-5.664	-6.935	11.619
ATOM	733	CA	THR	A	80	-3.658	-6.957	12.263
ATOM	734	C	THR	A	80	-3.490	-8.075	13.308
ATOM	735	O	THR	A	80	-4.447	-8.642	13.857
ATOM	736	CB	THR	A	80	-3.868	-5.572	12.927
ATOM	737	OG1	THR	A	80	-2.770	-5.303	13.787
ATOM	738	HG1	THR	A	80	-2.889	-4.412	14.225
ATOM	739	CG2	THR	A	80	-5.210	-5.464	13.678
ATOM	740	N	PRO	A	81	-2.243	-8.496	13.589
ATOM	741	CA	PRO	A	81	-1.986	-9.476	14.660
ATOM	742	C	PRO	A	81	-2.499	-8.952	16.001
ATOM	743	O	PRO	A	81	-2.944	-9.720	16.866
ATOM	744	CB	PRO	A	81	-0.444	-9.549	14.732
ATOM	745	CG	PRO	A	81	0.069	-8.951	13.429
ATOM	746	CD	PRO	A	81	-1.029	-8.105	12.842
ATOM	747	N	VAL	A	82	-2.474	-7.621	16.276
ATOM	748	H	VAL	A	82	-2.180	-6.975	15.571
ATOM	749	CA	VAL	A	82	-2.869	-7.091	17.591
ATOM	750	C	VAL	A	82	-3.605	-5.761	17.379
ATOM	751	O	VAL	A	82	-3.349	-5.004	16.429
ATOM	752	CB	VAL	A	82	-1.595	-6.858	18.443
ATOM	753	CG1	VAL	A	82	-0.650	-5.824	17.803
ATOM	754	CG2	VAL	A	82	-1.907	-6.418	19.890
ATOM	755	N	ASN	A	83	-4.548	-5.371	18.260
ATOM	756	H	ASN	A	83	-4.810	-5.981	19.007
ATOM	757	CA	ASN	A	83	-5.181	-4.067	18.123
ATOM	758	C	ASN	A	83	-4.195	-3.019	18.565
ATOM	759	O	ASN	A	83	-3.605	-3.064	19.665
ATOM	760	CB	ASN	A	83	-6.436	-3.942	18.982
ATOM	761	CG	ASN	A	83	-7.502	-4.930	18.631
ATOM	762	OD1	ASN	A	83	-7.899	-5.049	17.488
ATOM	763	ND2	ASN	A	83	-7.980	-5.662	19.628
ATOM	764	2HD2	ASN	A	83	-8.695	-6.341	19.459
ATOM	765	1HD2	ASN	A	83	-7.630	-5.541	20.557
ATOM	766	N	ILE	A	84	-4.007	-1.951	17.770
ATOM	767	H	ILE	A	84	-4.583	-1.827	16.962
ATOM	768	CA	ILE	A	84	-2.993	-0.954	18.032
ATOM	769	C	ILE	A	84	-3.679	0.387	18.114
ATOM	770	O	ILE	A	84	-4.460	0.797	17.240
ATOM	771	CB	ILE	A	84	-2.021	-0.922	16.833
ATOM	772	CG1	ILE	A	84	-1.162	-2.150	16.859
ATOM	773	CG2	ILE	A	84	-1.219	0.387	16.747
ATOM	774	CD1	ILE	A	84	-0.375	-2.360	15.579
ATOM	775	N	ILE	A	85	-3.471	1.155	19.203
ATOM	776	H	ILE	A	85	-2.972	0.781	19.985
ATOM	777	CA	ILE	A	85	-3.951	2.518	19.281
ATOM	778	C	ILE	A	85	-2.784	3.425	18.949
ATOM	779	O	ILE	A	85	-1.767	3.515	19.663
ATOM	780	CB	ILE	A	85	-4.522	2.825	20.676
ATOM	781	CG1	ILE	A	85	-5.673	1.865	21.050
ATOM	782	CG2	ILE	A	85	-5.000	4.274	20.716
ATOM	783	CD1	ILE	A	85	-6.828	1.808	20.059

FIG. 11 A-13

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ATOM	784	N	GLY	A	86	-2.820	4.123	17.792
ATOM	785	H	GLY	A	86	-3.637	4.087	17.217
ATOM	786	CA	GLY	A	86	-1.690	4.936	17.351
ATOM	787	C	GLY	A	86	-1.831	6.393	17.704
ATOM	788	O	GLY	A	86	-2.760	6.864	18.390
ATOM	789	N	ARG	A	87	-0.881	7.229	17.230
ATOM	790	H	ARG	A	87	-0.204	6.890	16.577
ATOM	791	CA	ARG	A	87	-0.810	8.623	17.643
ATOM	792	C	ARG	A	87	-2.027	9.445	17.277
ATOM	793	O	ARG	A	87	-2.365	10.430	17.963
ATOM	794	CB	ARG	A	87	0.450	9.275	17.057
ATOM	795	CG	ARG	A	87	1.735	8.496	17.205
ATOM	796	CD	ARG	A	87	2.762	8.916	16.207
ATOM	797	NE	ARG	A	87	3.875	7.961	16.117
ATOM	798	HE	ARG	A	87	4.035	7.353	16.895
ATOM	799	CZ	ARG	A	87	4.660	7.893	15.035
ATOM	800	NH1	ARG	A	87	4.463	8.675	13.975
ATOM	801	2HH1	ARG	A	87	3.712	9.335	13.974
ATOM	802	1HH1	ARG	A	87	5.066	8.602	13.181
ATOM	803	NH2	ARG	A	87	5.656	7.019	15.023
ATOM	804	1HH2	ARG	A	87	6.254	6.953	14.224
ATOM	805	2HH2	ARG	A	87	5.810	6.426	15.813
ATOM	806	N	ASN	A	88	-2.780	9.120	16.214
ATOM	807	H	ASN	A	88	-2.504	8.361	15.625
ATOM	808	CA	ASN	A	88	-4.015	9.860	15.890
ATOM	809	C	ASN	A	88	-4.963	9.921	17.069
ATOM	810	O	ASN	A	88	-5.613	10.954	17.345
ATOM	811	CB	ASN	A	88	-4.712	9.315	14.617
ATOM	812	CG	ASN	A	88	-5.475	8.001	14.827
ATOM	813	OD1	ASN	A	88	-4.922	6.996	15.245
ATOM	814	ND2	ASN	A	88	-6.758	7.998	14.506
ATOM	815	2HD2	ASN	A	88	-7.306	7.169	14.622
ATOM	816	1HD2	ASN	A	88	-7.190	8.824	14.145
ATOM	817	N	LEU	A	89	-5.130	8.847	17.848
ATOM	818	H	LEU	A	89	-4.637	8.002	17.640
ATOM	819	CA	LEU	A	89	-6.024	8.865	19.013
ATOM	820	C	LEU	A	89	-5.275	9.091	20.309
ATOM	821	O	LEU	A	89	-5.834	9.632	21.283
ATOM	822	CB	LEU	A	89	-6.840	7.592	19.140
ATOM	823	CG	LEU	A	89	-7.759	7.355	17.957
ATOM	824	CD1	LEU	A	89	-8.369	5.980	18.088
ATOM	825	CD2	LEU	A	89	-8.817	8.457	17.801
ATOM	826	N	LEU	A	90	-3.983	8.745	20.428
ATOM	827	H	LEU	A	90	-3.525	8.274	19.674
ATOM	828	CA	LEU	A	90	-3.242	9.057	21.664
ATOM	829	C	LEU	A	90	-3.155	10.555	21.932
ATOM	830	O	LEU	A	90	-3.202	11.020	23.092
ATOM	831	CB	LEU	A	90	-1.817	8.453	21.661
ATOM	832	CG	LEU	A	90	-1.766	6.914	21.587
ATOM	833	CD1	LEU	A	90	-0.343	6.494	21.396
ATOM	834	CD2	LEU	A	90	-2.339	6.230	22.812
ATOM	835	N	THR	A	91	-3.031	11.407	20.926
ATOM	836	H	THR	A	91	-2.982	11.063	19.988
ATOM	837	CA	THR	A	91	-2.964	12.834	21.155
ATOM	838	C	THR	A	91	-4.309	13.331	21.635
ATOM	839	O	THR	A	91	-4.422	14.315	22.398

FIG. 11 A-14
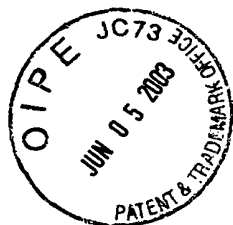
Heller Ehrman White & McAuliffe, LLP
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Title: Use of Computationally Derived Protein Structures of Genetic
Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
Serial No.: 09/709,905   Applicants: Ramnarayan *et al.*
Filed: 11/10/00   Attorney Docket No. 24737-1906C

|								
ATOM	840	CB	THR	A	91	-2.555	13.543	19.848
ATOM	841	OG1	THR	A	91	-3.459	13.214	18.802
ATOM	842	HG1	THR	A	91	-3.188	13.677	17.958
ATOM	843	CG2	THR	A	91	-1.153	13.122	19.395
ATOM	844	N	GLN	A	92	-5.435	12.704	21.258
ATOM	845	H	GLN	A	92	-5.379	11.892	20.677
ATOM	846	CA	GLN	A	92	-6.763	13.186	21.682
ATOM	847	C	GLN	A	92	-6.942	12.975	23.153
ATOM	848	O	GLN	A	92	-7.554	13.797	23.871
ATOM	849	CB	GLN	A	92	-7.890	12.479	20.964
ATOM	850	CG	GLN	A	92	-7.937	12.862	19.517
ATOM	851	CD	GLN	A	92	-9.251	12.515	18.886
ATOM	852	OE1	GLN	A	92	-10.270	12.424	19.546
ATOM	853	NE2	GLN	A	92	-9.202	12.323	17.588
ATOM	854	1HE2	GLN	A	92	-10.031	12.087	17.080
ATOM	855	2HE2	GLN	A	92	-8.336	12.411	17.097
ATOM	856	N	ILE	A	93	-6.472	11.846	23.721
ATOM	857	H	ILE	A	93	-6.014	11.160	23.155
ATOM	858	CA	ILE	A	93	-6.608	11.578	25.165
ATOM	859	C	ILE	A	93	-5.472	12.189	25.948
ATOM	860	O	ILE	A	93	-5.342	12.031	27.171
ATOM	861	CB	ILE	A	93	-6.820	10.073	25.484
ATOM	862	CG1	ILE	A	93	-5.536	9.221	25.286
ATOM	863	CG2	ILE	A	93	-8.022	9.486	24.735
ATOM	864	CD1	ILE	A	93	-5.754	7.740	25.693
ATOM	865	N	GLY	A	94	-4.594	12.993	25.330
ATOM	866	H	GLY	A	94	-4.617	13.079	24.334
ATOM	867	CA	GLY	A	94	-3.613	13.742	26.063
ATOM	868	C	GLY	A	94	-2.448	12.895	26.512
ATOM	869	O	GLY	A	94	-1.764	13.158	27.519
ATOM	870	N	CYS	A	95	-2.117	11.849	25.797
ATOM	871	H	CYS	A	95	-2.619	11.644	24.957
ATOM	872	CA	CYS	A	95	-1.036	10.994	26.214
ATOM	873	C	CYS	A	95	0.362	11.566	25.925
ATOM	874	O	CYS	A	95	0.588	12.254	24.907
ATOM	875	CB	CYS	A	95	-1.260	9.655	25.550
ATOM	876	SG	CYS	A	95	-0.254	8.307	26.125
ATOM	877	N	THR	A	96	1.346	11.297	26.803
ATOM	878	H	THR	A	96	1.135	10.738	27.618
ATOM	879	CA	THR	A	96	2.728	11.779	26.664
ATOM	880	C	THR	A	96	3.729	10.784	27.264
ATOM	881	O	THR	A	96	3.498	10.249	28.345
ATOM	882	CB	THR	A	96	2.925	13.154	27.346
ATOM	883	OG1	THR	A	96	2.594	13.109	28.721
ATOM	884	HG1	THR	A	96	2.784	13.966	29.109
ATOM	885	CG2	THR	A	96	2.139	14.300	26.698
ATOM	886	N	LEU	A	97	4.882	10.603	26.599
ATOM	887	H	LEU	A	97	5.016	11.071	25.714
ATOM	888	CA	LEU	A	97	6.040	9.910	27.166
ATOM	889	C	LEU	A	97	6.751	10.824	28.175
ATOM	890	O	LEU	A	97	6.705	12.046	28.044
ATOM	891	CB	LEU	A	97	7.013	9.497	26.049
ATOM	892	CG	LEU	A	97	6.452	8.449	25.065
ATOM	893	CD1	LEU	A	97	7.360	8.355	23.828
ATOM	894	CD2	LEU	A	97	6.345	7.065	25.724
ATOM	895	N	ASN	A	98	7.412	10.221	29.175

FIG. 11A-15

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Filed: 11/10/00   Attorney Docket No. 24737-1906C

```
ATOM    896   H    ASN A  98      7.413    9.212   29.205
ATOM    897   CA   ASN A  98      8.065   10.897   30.292
ATOM    898   C    ASN A  98      9.220   10.029   30.800
ATOM    899   O    ASN A  98      8.995    9.079   31.550
ATOM    900   CB   ASN A  98      7.057   11.177   31.423
ATOM    901   CG   ASN A  98      6.084   12.305   31.083
ATOM    902   OD1  ASN A  98      4.983   12.062   30.594
ATOM    903   ND2  ASN A  98      6.493   13.549   31.342
ATOM    904  2HD2  ASN A  98      5.888   14.331   31.136
ATOM    905  1HD2  ASN A  98      7.406   13.707   31.742
ATOM    906   N    LEU A  99     10.451   10.369   30.389
ATOM    907   H    LEU A  99     10.547   11.177   29.792
ATOM    908   CA   LEU A  99     11.679    9.620   30.666
ATOM    909   C    LEU A  99     12.711   10.437   31.454
ATOM    910   O    LEU A  99     12.487   11.652   31.651
ATOM    911   CB   LEU A  99     12.233    8.989   29.369
ATOM    912   CG   LEU A  99     12.833    9.873   28.248
ATOM    913   CD1  LEU A  99     11.876   10.947   27.705
ATOM    914   CD2  LEU A  99     14.183   10.505   28.623
ATOM    915   OXT  LEU A  99     13.716    9.819   31.869
TER
ATOM    916   N    PRO B   1     12.600   14.237   30.106
ATOM    917   CA   PRO B   1     11.842   15.268   29.363
ATOM    918   C    PRO B   1     10.430   14.773   29.138
ATOM    919   O    PRO B   1     10.054   13.695   29.618
ATOM    920   CB   PRO B   1     12.622   15.412   28.035
ATOM    921   CG   PRO B   1     13.817   14.470   28.131
ATOM    922   CD   PRO B   1     13.966   14.227   29.603
ATOM    923  1H    PRO B   1     12.175   13.343   29.964
ATOM    924  2H    PRO B   1     12.594   14.457   31.081
ATOM    925   N    GLN B   2      9.513   15.542   28.523
ATOM    926   H    GLN B   2      9.751   16.474   28.251
ATOM    927   CA   GLN B   2      8.186   15.058   28.242
ATOM    928   C    GLN B   2      8.066   15.151   26.749
ATOM    929   O    GLN B   2      8.523   16.140   26.133
ATOM    930   CB   GLN B   2      7.155   15.976   28.856
ATOM    931   CG   GLN B   2      5.739   15.732   28.373
ATOM    932   CD   GLN B   2      4.744   16.365   29.284
ATOM    933   OE1  GLN B   2      4.628   15.962   30.431
ATOM    934   NE2  GLN B   2      4.024   17.367   28.784
ATOM    935  1HE2  GLN B   2      3.341   17.830   29.349
ATOM    936  2HE2  GLN B   2      4.160   17.665   27.839
ATOM    937   N    ILE B   3      7.499   14.176   26.036
ATOM    938   H    ILE B   3      7.102   13.386   26.504
ATOM    939   CA   ILE B   3      7.435   14.216   24.601
ATOM    940   C    ILE B   3      5.956   14.097   24.184
ATOM    941   O    ILE B   3      5.150   13.290   24.710
ATOM    942   CB   ILE B   3      8.299   13.058   24.029
ATOM    943   CG1  ILE B   3      9.743   13.232   24.534
ATOM    944   CG2  ILE B   3      8.269   12.985   22.496
ATOM    945   CD1  ILE B   3     10.621   12.068   24.143
ATOM    946   N    THR B   4      5.462   15.108   23.453
ATOM    947   H    THR B   4      6.046   15.887   23.226
ATOM    948   CA   THR B   4      4.107   15.115   22.976
ATOM    949   C    THR B   4      4.039   14.193   21.765
ATOM    950   O    THR B   4      5.066   13.755   21.203
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FIG. 11 A-16
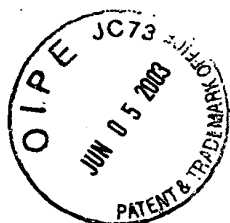
Heller Ehrman White & McAuliffe, LLP
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Title: Use of Computationally Derived Protein Structures of Genetic
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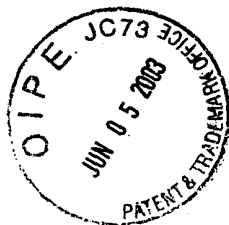Serial No.: 09/709,905   Applicants: Ramnarayan *et al.*
Filed: 11/10/00   Attorney Docket No. 24737-1906C

| ATOM	951	CB	THR	B	4	3.616	16.548	22.647
ATOM	952	OG1	THR	B	4	4.450	17.157	21.645
ATOM	953	HG1	THR	B	4	4.123	18.080	21.442
ATOM	954	CG2	THR	B	4	3.644	17.454	23.876
ATOM	955	N	LEU	B	5	2.872	13.781	21.324
ATOM	956	H	LEU	B	5	2.033	14.151	21.723
ATOM	957	CA	LEU	B	5	2.837	12.795	20.265
ATOM	958	C	LEU	B	5	2.183	13.415	19.047
ATOM	959	O	LEU	B	5	1.677	12.720	18.142
ATOM	960	CB	LEU	B	5	2.093	11.577	20.762
ATOM	961	CG	LEU	B	5	2.819	10.856	21.892
ATOM	962	CD1	LEU	B	5	1.889	9.885	22.602
ATOM	963	CD2	LEU	B	5	4.108	10.159	21.416
ATOM	964	N	TRP	B	6	2.209	14.742	18.880
ATOM	965	H	TRP	B	6	2.601	15.323	19.593
ATOM	966	CA	TRP	B	6	1.683	15.364	17.690
ATOM	967	C	TRP	B	6	2.581	14.978	16.509
ATOM	968	O	TRP	B	6	2.159	14.851	15.349
ATOM	969	CB	TRP	B	6	1.587	16.879	17.833
ATOM	970	CG	TRP	B	6	0.652	17.339	18.921
ATOM	971	CD1	TRP	B	6	0.955	17.584	20.232
ATOM	972	CD2	TRP	B	6	-0.750	17.612	18.783
ATOM	973	NE1	TRP	B	6	-0.167	17.989	20.913
ATOM	974	HE1	TRP	B	6	-0.217	18.230	21.882
ATOM	975	CE2	TRP	B	6	-1.224	18.013	20.048
ATOM	976	CE3	TRP	B	6	-1.637	17.550	17.709
ATOM	977	CZ2	TRP	B	6	-2.544	18.352	20.266
ATOM	978	CZ3	TRP	B	6	-2.947	17.885	17.921
ATOM	979	CH2	TRP	B	6	-3.394	18.281	19.185
ATOM	980	N	GLN	B	7	3.896	14.809	16.738
ATOM	981	H	GLN	B	7	4.267	14.985	17.650
ATOM	982	CA	GLN	B	7	4.794	14.376	15.689
ATOM	983	C	GLN	B	7	5.361	13.043	16.096
ATOM	984	O	GLN	B	7	5.221	12.586	17.243
ATOM	985	CB	GLN	B	7	5.880	15.430	15.505
ATOM	986	CG	GLN	B	7	5.353	16.704	14.804
ATOM	987	CD	GLN	B	7	6.197	17.912	15.137
ATOM	988	OE1	GLN	B	7	7.400	17.802	15.404
ATOM	989	NE2	GLN	B	7	5.553	19.083	15.121
ATOM	990	1HE2	GLN	B	7	6.040	19.931	15.330
ATOM	991	2HE2	GLN	B	7	4.579	19.121	14.900
ATOM	992	N	ARG	B	8	5.979	12.274	15.189
ATOM	993	H	ARG	B	8	6.073	12.597	14.247
ATOM	994	CA	ARG	B	8	6.505	10.985	15.573
ATOM	995	C	ARG	B	8	7.577	11.198	16.610
ATOM	996	O	ARG	B	8	8.395	12.130	16.515
ATOM	997	CB	ARG	B	8	7.092	10.238	14.384
ATOM	998	CG	ARG	B	8	6.132	10.018	13.237
ATOM	999	CD	ARG	B	8	6.802	9.402	12.046
ATOM	1000	NE	ARG	B	8	5.846	9.005	11.023
ATOM	1001	HE	ARG	B	8	4.872	9.080	11.237
ATOM	1002	CZ	ARG	B	8	6.217	8.552	9.828
ATOM	1003	NH1	ARG	B	8	7.496	8.442	9.486
ATOM	1004	2HH1	ARG	B	8	8.211	8.703	10.134
ATOM	1005	1HH1	ARG	B	8	7.744	8.098	8.580
ATOM	1006	NH2	ARG	B	8	5.279	8.202	8.952

FIG. 11A-17

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| ATOM	1007	1HH2	ARG	B	8	5.540	7.860	8.050
ATOM	1008	2HH2	ARG	B	8	4.312	8.281	9.196
ATOM	1009	N	PRO	B	9	7.663	10.381	17.682
ATOM	1010	CA	PRO	B	9	8.666	10.587	18.746
ATOM	1011	C	PRO	B	9	10.065	10.196	18.315
ATOM	1012	O	PRO	B	9	10.678	9.215	18.778
ATOM	1013	CB	PRO	B	9	8.148	9.682	19.878
ATOM	1014	CG	PRO	B	9	7.315	8.607	19.206
ATOM	1015	CD	PRO	B	9	6.708	9.323	18.004
ATOM	1016	N	LEU	B	10	10.685	10.969	17.400
ATOM	1017	H	LEU	B	10	10.201	11.746	16.998
ATOM	1018	CA	LEU	B	10	12.040	10.706	16.978
ATOM	1019	C	LEU	B	10	12.976	11.498	17.850
ATOM	1020	O	LEU	B	10	12.880	12.733	18.018
ATOM	1021	CB	LEU	B	10	12.250	11.170	15.554
ATOM	1022	CG	LEU	B	10	11.427	10.386	14.551
ATOM	1023	CD1	LEU	B	10	11.385	11.175	13.276
ATOM	1024	CD2	LEU	B	10	11.956	8.947	14.355
ATOM	1025	N	VAL	B	11	14.030	10.843	18.384
ATOM	1026	H	VAL	B	11	14.148	9.866	18.206
ATOM	1027	CA	VAL	B	11	15.018	11.517	19.223
ATOM	1028	C	VAL	B	11	16.400	11.111	18.740
ATOM	1029	O	VAL	B	11	16.581	10.201	17.911
ATOM	1030	CB	VAL	B	11	14.857	11.100	20.699
ATOM	1031	CG1	VAL	B	11	13.514	11.586	21.293
ATOM	1032	CG2	VAL	B	11	15.038	9.573	20.903
ATOM	1033	N	THR	B	12	17.485	11.739	19.232
ATOM	1034	H	THR	B	12	17.370	12.507	19.862
ATOM	1035	CA	THR	B	12	18.843	11.325	18.868
ATOM	1036	C	THR	B	12	19.377	10.284	19.837
ATOM	1037	O	THR	B	12	19.237	10.352	21.082
ATOM	1038	CB	THR	B	12	19.830	12.520	18.820
ATOM	1039	OG1	THR	B	12	19.389	13.483	17.876
ATOM	1040	HG1	THR	B	12	20.028	14.252	17.848
ATOM	1041	CG2	THR	B	12	21.234	12.075	18.399
ATOM	1042	N	ILE	B	13	20.044	9.234	19.338
ATOM	1043	H	ILE	B	13	20.135	9.130	18.348
ATOM	1044	CA	ILE	B	13	20.641	8.239	20.176
ATOM	1045	C	ILE	B	13	22.119	8.226	19.855
ATOM	1046	O	ILE	B	13	22.579	8.817	18.865
ATOM	1047	CB	ILE	B	13	19.993	6.870	19.879
ATOM	1048	CG1	ILE	B	13	20.192	6.464	18.415
ATOM	1049	CG2	ILE	B	13	18.482	6.893	20.206
ATOM	1050	CD1	ILE	B	13	19.829	5.035	18.106
ATOM	1051	N	LYS	B	14	22.973	7.618	20.661
ATOM	1052	H	LYS	B	14	22.652	7.243	21.531
ATOM	1053	CA	LYS	B	14	24.364	7.480	20.317
ATOM	1054	C	LYS	B	14	24.680	6.029	20.477
ATOM	1055	O	LYS	B	14	24.353	5.353	21.484
ATOM	1056	CB	LYS	B	14	25.266	8.263	21.242
ATOM	1057	CG	LYS	B	14	24.947	9.729	21.236
ATOM	1058	CD	LYS	B	14	25.664	10.498	22.339
ATOM	1059	CE	LYS	B	14	26.758	11.441	21.807
ATOM	1060	NZ	LYS	B	14	28.026	10.781	21.440
ATOM	1061	1HZ	LYS	B	14	28.674	11.466	21.107
ATOM	1062	3HZ	LYS	B	14	27.855	10.107	20.722

FIG. 11A-18
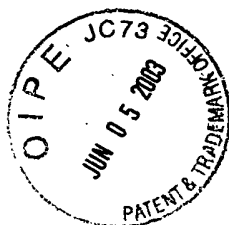
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ATOM	1063	2HZ	LYS	B	14	28.408	10.323	22.243
ATOM	1064	N	ILE	B	15	25.214	5.390	19.425
ATOM	1065	H	ILE	B	15	25.434	5.901	18.594
ATOM	1066	CA	ILE	B	15	25.489	3.989	19.434
ATOM	1067	C	ILE	B	15	26.832	3.981	18.750
ATOM	1068	O	ILE	B	15	27.104	4.869	17.933
ATOM	1069	CB	ILE	B	15	24.435	3.220	18.606
ATOM	1070	CG1	ILE	B	15	24.893	1.824	18.347
ATOM	1071	CG2	ILE	B	15	24.048	3.977	17.309
ATOM	1072	CD1	ILE	B	15	23.830	0.996	17.645
ATOM	1073	N	GLY	B	16	27.812	3.212	19.202
ATOM	1074	H	GLY	B	16	27.623	2.535	19.913
ATOM	1075	CA	GLY	B	16	29.175	3.336	18.677
ATOM	1076	C	GLY	B	16	29.771	4.754	18.619
ATOM	1077	O	GLY	B	16	30.737	4.970	17.902
ATOM	1078	N	GLY	B	17	29.273	5.791	19.335
ATOM	1079	H	GLY	B	17	28.453	5.660	19.892
ATOM	1080	CA	GLY	B	17	29.924	7.105	19.302
ATOM	1081	C	GLY	B	17	29.468	8.043	18.176
ATOM	1082	O	GLY	B	17	29.984	9.155	17.933
ATOM	1083	N	GLN	B	18	28.433	7.621	17.411
ATOM	1084	H	GLN	B	18	28.046	6.711	17.560
ATOM	1085	CA	GLN	B	18	27.834	8.449	16.348
ATOM	1086	C	GLN	B	18	26.407	8.755	16.736
ATOM	1087	O	GLN	B	18	25.678	7.953	17.353
ATOM	1088	CB	GLN	B	18	27.810	7.645	15.045
ATOM	1089	CG	GLN	B	18	27.247	6.204	15.146
ATOM	1090	CD	GLN	B	18	27.572	5.333	13.924
ATOM	1091	OE1	GLN	B	18	26.771	4.501	13.464
ATOM	1092	NE2	GLN	B	18	28.766	5.531	13.393
ATOM	1093	1HE2	GLN	B	18	29.057	5.005	12.594
ATOM	1094	2HE2	GLN	B	18	29.388	6.209	13.786
ATOM	1095	N	LEU	B	19	25.873	9.933	16.337
ATOM	1096	H	LEU	B	19	26.446	10.602	15.863
ATOM	1097	CA	LEU	B	19	24.467	10.267	16.578
ATOM	1098	C	LEU	B	19	23.633	9.622	15.490
ATOM	1099	O	LEU	B	19	23.912	9.707	14.284
ATOM	1100	CB	LEU	B	19	24.207	11.777	16.457
ATOM	1101	CG	LEU	B	19	24.857	12.756	17.454
ATOM	1102	CD1	LEU	B	19	24.739	12.335	18.880
ATOM	1103	CD2	LEU	B	19	26.299	13.072	17.130
ATOM	1104	N	LYS	B	20	22.450	9.085	15.850
ATOM	1105	H	LYS	B	20	22.242	8.948	16.819
ATOM	1106	CA	LYS	B	20	21.472	8.702	14.867
ATOM	1107	C	LYS	B	20	20.121	9.105	15.417
ATOM	1108	O	LYS	B	20	19.957	9.572	16.569
ATOM	1109	CB	LYS	B	20	21.496	7.200	14.560
ATOM	1110	CG	LYS	B	20	22.904	6.653	14.507
ATOM	1111	CD	LYS	B	20	23.052	5.366	13.677
ATOM	1112	CE	LYS	B	20	23.069	5.603	12.145
ATOM	1113	NZ	LYS	B	20	23.893	6.758	11.699
ATOM	1114	1HZ	LYS	B	20	23.847	6.836	10.703
ATOM	1115	3HZ	LYS	B	20	24.843	6.617	11.978
ATOM	1116	2HZ	LYS	B	20	23.544	7.597	12.116
ATOM	1117	N	GLU	B	21	19.068	9.022	14.591
ATOM	1118	H	GLU	B	21	19.200	8.712	13.650

FIG. 11A-19
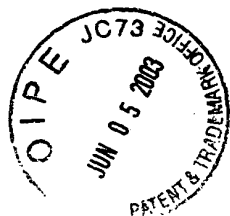
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Title: Use of Computationally Derived Protein Structures of Genetic
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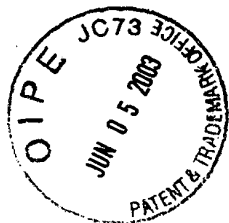Serial No.: 09/709,905   Applicants: Ramnarayan *et al.*
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ATOM	1119	CA	GLU	B	21	17.735	9.366	15.008
ATOM	1120	C	GLU	B	21	16.937	8.095	15.119
ATOM	1121	O	GLU	B	21	17.117	7.103	14.376
ATOM	1122	CB	GLU	B	21	17.143	10.314	13.983
ATOM	1123	CG	GLU	B	21	15.714	10.706	14.162
ATOM	1124	CD	GLU	B	21	15.304	11.607	13.036
ATOM	1125	OE1	GLU	B	21	14.971	11.051	11.957
ATOM	1126	OE2	GLU	B	21	15.338	12.854	13.174
ATOM	1127	N	ALA	B	22	16.025	7.999	16.072
ATOM	1128	H	ALA	B	22	15.825	8.792	16.648
ATOM	1129	CA	ALA	B	22	15.300	6.783	16.315
ATOM	1130	C	ALA	B	22	13.981	7.132	16.952
ATOM	1131	O	ALA	B	22	13.756	8.153	17.632
ATOM	1132	CB	ALA	B	22	16.095	5.865	17.235
ATOM	1133	N	LEU	B	23	12.994	6.230	16.743
ATOM	1134	H	LEU	B	23	13.195	5.379	16.257
ATOM	1135	CA	LEU	B	23	11.639	6.408	17.180
ATOM	1136	C	LEU	B	23	11.476	5.740	18.534
ATOM	1137	O	LEU	B	23	11.814	4.564	18.746
ATOM	1138	CB	LEU	B	23	10.775	5.665	16.192
ATOM	1139	CG	LEU	B	23	9.267	5.810	16.237
ATOM	1140	CD1	LEU	B	23	8.807	7.142	15.664
ATOM	1141	CD2	LEU	B	23	8.648	4.625	15.482
ATOM	1142	N	LEU	B	24	10.948	6.455	19.553
ATOM	1143	H	LEU	B	24	10.775	7.433	19.435
ATOM	1144	CA	LEU	B	24	10.613	5.838	20.849
ATOM	1145	C	LEU	B	24	9.271	5.160	20.687
ATOM	1146	O	LEU	B	24	8.208	5.764	20.418
ATOM	1147	CB	LEU	B	24	10.564	6.878	21.971
ATOM	1148	CG	LEU	B	24	11.828	7.750	22.075
ATOM	1149	CD1	LEU	B	24	11.580	8.859	23.077
ATOM	1150	CD2	LEU	B	24	13.099	6.955	22.388
ATOM	1151	N	ASP	B	25	9.246	3.822	20.809
ATOM	1152	H	ASP	B	25	10.025	3.347	21.218
ATOM	1153	CA	ASP	B	25	8.122	3.030	20.366
ATOM	1154	C	ASP	B	25	7.637	2.136	21.484
ATOM	1155	O	ASP	B	25	8.189	1.048	21.759
ATOM	1156	CB	ASP	B	25	8.613	2.196	19.189
ATOM	1157	CG	ASP	B	25	7.528	1.421	18.511
ATOM	1158	OD1	ASP	B	25	6.422	1.339	19.058
ATOM	1159	OD2	ASP	B	25	7.800	0.897	17.426
ATOM	1160	N	THR	B	26	6.547	2.465	22.157
ATOM	1161	H	THR	B	26	6.067	3.314	21.938
ATOM	1162	CA	THR	B	26	6.025	1.621	23.212
ATOM	1163	C	THR	B	26	5.347	0.369	22.694
ATOM	1164	O	THR	B	26	4.976	-0.550	23.451
ATOM	1165	CB	THR	B	26	5.027	2.389	24.046
ATOM	1166	OG1	THR	B	26	3.927	2.853	23.239
ATOM	1167	HG1	THR	B	26	3.277	3.359	23.806
ATOM	1168	CG2	THR	B	26	5.703	3.603	24.650
ATOM	1169	N	GLY	B	27	5.090	0.245	21.382
ATOM	1170	H	GLY	B	27	5.341	0.983	20.756
ATOM	1171	CA	GLY	B	27	4.457	-0.938	20.867
ATOM	1172	C	GLY	B	27	5.475	-1.992	20.458
ATOM	1173	O	GLY	B	27	5.121	-3.108	20.055
ATOM	1174	N	ALA	B	28	6.792	-1.717	20.495

FIG. 11 A-20

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ATOM	1175	H	ALA	B	28	7.104	-0.832	20.841
ATOM	1176	CA	ALA	B	28	7.800	-2.690	20.037
ATOM	1177	C	ALA	B	28	8.371	-3.444	21.259
ATOM	1178	O	ALA	B	28	8.840	-2.807	22.213
ATOM	1179	CB	ALA	B	28	8.924	-1.936	19.358
ATOM	1180	N	ASP	B	29	8.459	-4.787	21.289
ATOM	1181	H	ASP	B	29	8.082	-5.325	20.535
ATOM	1182	CA	ASP	B	29	9.121	-5.441	22.452
ATOM	1183	C	ASP	B	29	10.608	-5.219	22.404
ATOM	1184	O	ASP	B	29	11.345	-5.264	23.412
ATOM	1185	CB	ASP	B	29	8.965	-6.975	22.447
ATOM	1186	CG	ASP	B	29	7.551	-7.477	22.774
ATOM	1187	OD1	ASP	B	29	6.683	-6.693	23.169
ATOM	1188	OD2	ASP	B	29	7.350	-8.686	22.616
ATOM	1189	N	ASP	B	30	11.164	-5.157	21.171
ATOM	1190	H	ASP	B	30	10.577	-5.063	20.367
ATOM	1191	CA	ASP	B	30	12.609	-5.217	20.880
ATOM	1192	C	ASP	B	30	13.048	-3.886	20.335
ATOM	1193	O	ASP	B	30	12.269	-3.055	19.817
ATOM	1194	CB	ASP	B	30	12.833	-6.226	19.735
ATOM	1195	CG	ASP	B	30	12.477	-7.675	20.099
ATOM	1196	OD1	ASP	B	30	13.197	-8.272	20.908
ATOM	1197	OD2	ASP	B	30	11.494	-8.237	19.569
ATOM	1198	N	THR	B	31	14.387	-3.692	20.227
ATOM	1199	H	THR	B	31	15.018	-4.380	20.586
ATOM	1200	CA	THR	B	31	14.981	-2.530	19.614
ATOM	1201	C	THR	B	31	15.578	-2.979	18.260
ATOM	1202	O	THR	B	31	16.246	-4.020	18.123
ATOM	1203	CB	THR	B	31	16.036	-2.004	20.557
ATOM	1204	OG1	THR	B	31	15.378	-1.376	21.645
ATOM	1205	HG1	THR	B	31	16.052	-1.016	22.290
ATOM	1206	CG2	THR	B	31	16.944	-0.960	19.904
ATOM	1207	N	VAL	B	32	15.237	-2.283	17.150
ATOM	1208	H	VAL	B	32	14.703	-1.442	17.237
ATOM	1209	CA	VAL	B	32	15.626	-2.722	15.806
ATOM	1210	C	VAL	B	32	16.303	-1.566	15.132
ATOM	1211	O	VAL	B	32	15.779	-0.428	14.995
ATOM	1212	CB	VAL	B	32	14.407	-3.126	14.964
ATOM	1213	CG1	VAL	B	32	14.820	-3.703	13.596
ATOM	1214	CG2	VAL	B	32	13.556	-4.102	15.703
ATOM	1215	N	LEU	B	33	17.563	-1.756	14.720
ATOM	1216	H	LEU	B	33	17.984	-2.658	14.814
ATOM	1217	CA	LEU	B	33	18.347	-0.697	14.138
ATOM	1218	C	LEU	B	33	18.610	-1.009	12.685
ATOM	1219	O	LEU	B	33	18.685	-2.162	12.205
ATOM	1220	CB	LEU	B	33	19.679	-0.628	14.856
ATOM	1221	CG	LEU	B	33	19.698	0.363	16.031
ATOM	1222	CD1	LEU	B	33	18.425	0.321	16.891
ATOM	1223	CD2	LEU	B	33	20.929	0.179	16.889
ATOM	1224	N	GLU	B	34	18.786	0.078	11.899
ATOM	1225	H	GLU	B	34	18.619	0.991	12.271
ATOM	1226	CA	GLU	B	34	19.218	0.041	10.488
ATOM	1227	C	GLU	B	34	20.478	-0.774	10.399
ATOM	1228	O	GLU	B	34	21.374	-0.835	11.272
ATOM	1229	CB	GLU	B	34	19.536	1.460	9.996
ATOM	1230	CG	GLU	B	34	20.722	2.088	10.761

FIG. 11A-21

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| ATOM	1231	CD	GLU	B	34	21.085	3.512	10.314
ATOM	1232	OE1	GLU	B	34	20.285	4.466	10.500
ATOM	1233	OE2	GLU	B	34	22.211	3.703	9.775
ATOM	1234	N	GLU	B	35	20.673	-1.367	9.205
ATOM	1235	H	GLU	B	35	20.011	-1.227	8.468
ATOM	1236	CA	GLU	B	35	21.802	-2.205	8.930
ATOM	1237	C	GLU	B	35	23.096	-1.520	9.321
ATOM	1238	O	GLU	B	35	23.391	-0.379	8.916
ATOM	1239	CB	GLU	B	35	21.741	-2.479	7.439
ATOM	1240	CG	GLU	B	35	22.795	-3.380	6.883
ATOM	1241	CD	GLU	B	35	22.987	-4.587	7.744
ATOM	1242	OE1	GLU	B	35	21.980	-5.258	8.118
ATOM	1243	OE2	GLU	B	35	24.149	-4.860	8.048
ATOM	1244	N	MET	B	36	23.926	-2.106	10.157
ATOM	1245	H	MET	B	36	23.654	-2.953	10.613
ATOM	1246	CA	MET	B	36	25.232	-1.559	10.441
ATOM	1247	C	MET	B	36	26.146	-2.687	10.815
ATOM	1248	O	MET	B	36	25.731	-3.783	11.257
ATOM	1249	CB	MET	B	36	25.251	-0.424	11.497
ATOM	1250	CG	MET	B	36	24.626	-0.724	12.881
ATOM	1251	SD	MET	B	36	24.722	0.719	13.988
ATOM	1252	CE	MET	B	36	23.132	1.586	13.692
ATOM	1253	N	SER	B	37	27.441	-2.551	10.593
ATOM	1254	H	SER	B	37	27.783	-1.726	10.144
ATOM	1255	CA	SER	B	37	28.321	-3.608	11.011
ATOM	1256	C	SER	B	37	28.721	-3.352	12.442
ATOM	1257	O	SER	B	37	29.402	-2.369	12.788
ATOM	1258	CB	SER	B	37	29.567	-3.622	10.109
ATOM	1259	OG	SER	B	37	29.231	-3.908	8.750
ATOM	1260	HG	SER	B	37	30.057	-3.911	8.187
ATOM	1261	N	LEU	B	38	28.469	-4.295	13.366
ATOM	1262	H	LEU	B	38	27.948	-5.123	13.117
ATOM	1263	CA	LEU	B	38	29.073	-4.232	14.714
ATOM	1264	C	LEU	B	38	30.132	-5.342	14.895
ATOM	1265	O	LEU	B	38	30.070	-6.357	14.197
ATOM	1266	CB	LEU	B	38	27.986	-4.237	15.802
ATOM	1267	CG	LEU	B	38	27.005	-3.039	15.750
ATOM	1268	CD1	LEU	B	38	25.885	-3.214	16.788
ATOM	1269	CD2	LEU	B	38	27.707	-1.696	16.017
ATOM	1270	N	PRO	B	39	31.119	-5.160	15.804
ATOM	1271	CA	PRO	B	39	32.199	-6.116	16.052
ATOM	1272	C	PRO	B	39	31.767	-7.223	17.028
ATOM	1273	O	PRO	B	39	31.448	-6.942	18.185
ATOM	1274	CB	PRO	B	39	33.347	-5.276	16.625
ATOM	1275	CG	PRO	B	39	32.634	-4.148	17.370
ATOM	1276	CD	PRO	B	39	31.385	-3.916	16.523
ATOM	1277	N	GLY	B	40	31.770	-8.481	16.559
ATOM	1278	H	GLY	B	40	32.036	-8.641	15.598
ATOM	1279	CA	GLY	B	40	31.420	-9.658	17.353
ATOM	1280	C	GLY	B	40	30.679	-10.723	16.539
ATOM	1281	O	GLY	B	40	30.647	-10.671	15.308
ATOM	1282	N	LYS	B	41	30.098	-11.699	17.255
ATOM	1283	H	LYS	B	41	30.164	-11.656	18.261
ATOM	1284	CA	LYS	B	41	29.399	-12.861	16.702
ATOM	1285	C	LYS	B	41	27.971	-12.923	17.245
ATOM	1286	O	LYS	B	41	27.743	-12.700	18.436

FIG. 11 A-22

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Title: Use of Computationally Derived Protein Structures of Genetic
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Filed: 11/10/00   Attorney Docket No. 24737-1906C

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ATOM    1287   CB    LYS  B   41      30.154  -14.152   17.048
ATOM    1288   CG    LYS  B   41      31.537  -14.221   16.384
ATOM    1289   CD    LYS  B   41      32.192  -15.580   16.651
ATOM    1290   CE    LYS  B   41      33.566  -15.642   15.983
ATOM    1291   NZ    LYS  B   41      34.198  -16.956   16.183
ATOM    1292  1HZ    LYS  B   41      35.102  -16.968   15.732
ATOM    1293  3HZ    LYS  B   41      33.612  -17.674   15.782
ATOM    1294  2HZ    LYS  B   41      34.312  -17.128   17.172
ATOM    1295   N     TRP  B   42      27.018  -13.228   16.351
ATOM    1296   H     TRP  B   42      27.307  -13.458   15.411
ATOM    1297   CA    TRP  B   42      25.597  -12.929   16.521
ATOM    1298   C     TRP  B   42      24.723  -14.179   16.405
ATOM    1299   O     TRP  B   42      25.210  -15.277   16.131
ATOM    1300   CB    TRP  B   42      25.192  -11.856   15.491
ATOM    1301   CG    TRP  B   42      26.127  -10.687   15.390
ATOM    1302   CD1   TRP  B   42      26.651  -10.197   14.244
ATOM    1303   CD2   TRP  B   42      26.739   -9.913   16.467
ATOM    1304   NE1   TRP  B   42      27.548   -9.191   14.533
ATOM    1305   HE1   TRP  B   42      28.067   -8.702   13.818
ATOM    1306   CE2   TRP  B   42      27.664   -8.995   15.893
ATOM    1307   CE3   TRP  B   42      26.640   -9.923   17.875
ATOM    1308   CZ2   TRP  B   42      28.443   -8.136   16.680
ATOM    1309   CZ3   TRP  B   42      27.426   -9.075   18.673
ATOM    1310   CH2   TRP  B   42      28.318   -8.171   18.077
ATOM    1311   N     LYS  B   43      23.416  -13.980   16.617
ATOM    1312   H     LYS  B   43      23.105  -13.044   16.840
ATOM    1313   CA    LYS  B   43      22.378  -14.995   16.526
ATOM    1314   C     LYS  B   43      21.368  -14.507   15.478
ATOM    1315   O     LYS  B   43      20.743  -13.472   15.706
ATOM    1316   CB    LYS  B   43      21.694  -15.196   17.893
ATOM    1317   CG    LYS  B   43      22.641  -15.623   19.034
ATOM    1318   CD    LYS  B   43      22.409  -14.814   20.323
ATOM    1319   CE    LYS  B   43      22.767  -13.327   20.182
ATOM    1320   NZ    LYS  B   43      24.214  -13.113   20.015
ATOM    1321  1HZ    LYS  B   43      24.400  -12.125   19.924
ATOM    1322  3HZ    LYS  B   43      24.532  -13.593   19.185
ATOM    1323  2HZ    LYS  B   43      24.702  -13.476   20.821
ATOM    1324   N     PRO  B   44      21.175  -15.204   14.341
ATOM    1325   CA    PRO  B   44      20.139  -14.835   13.382
ATOM    1326   C     PRO  B   44      18.765  -14.997   14.044
ATOM    1327   O     PRO  B   44      18.573  -15.902   14.860
ATOM    1328   CB    PRO  B   44      20.341  -15.761   12.180
ATOM    1329   CG    PRO  B   44      20.999  -16.999   12.787
ATOM    1330   CD    PRO  B   44      21.837  -16.434   13.933
ATOM    1331   N     LYS  B   45      17.825  -14.101   13.712
ATOM    1332   H     LYS  B   45      17.994  -13.483   12.944
ATOM    1333   CA    LYS  B   45      16.523  -14.088   14.339
ATOM    1334   C     LYS  B   45      15.519  -13.590   13.329
ATOM    1335   O     LYS  B   45      15.829  -12.838   12.379
ATOM    1336   CB    LYS  B   45      16.558  -13.149   15.560
ATOM    1337   CG    LYS  B   45      15.469  -13.442   16.579
ATOM    1338   CD    LYS  B   45      15.256  -12.254   17.501
ATOM    1339   CE    LYS  B   45      14.131  -12.461   18.469
ATOM    1340   NZ    LYS  B   45      14.549  -13.442   19.474
ATOM    1341  1HZ    LYS  B   45      13.805  -13.588   20.126
ATOM    1342  3HZ    LYS  B   45      15.355  -13.101   19.958
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FIG. 11A-23
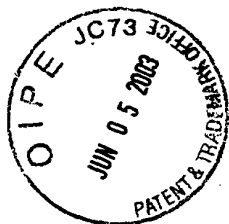
Heller Ehrman White & McAuliffe, LLP
Sheet 25 of 33
Title: Use of Computationally Derived Protein Structures of Genetic
Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
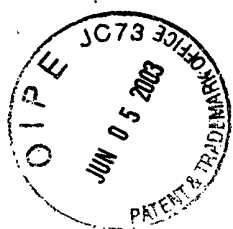Serial No.: 09/709,905   Applicants: Ramnarayan *et al.*
Filed: 11/10/00   Attorney Docket No. 24737-1906C

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ATOM   1343 2HZ LYS B   45   14.772 -14.306   19.023
ATOM   1344 N   MET B   46   14.240 -14.005   13.416
ATOM   1345 H   MET B   46   13.991 -14.705   14.085
ATOM   1346 CA   MET B   46   13.203 -13.472   12.570
ATOM   1347 C   MET B   46   12.291 -12.623   13.425
ATOM   1348 O   MET B   46   11.782 -13.063   14.471
ATOM   1349 CB   MET B   46   12.383 -14.616   12.016
ATOM   1350 CG   MET B   46   13.153 -15.586   11.187
ATOM   1351 SD   MET B   46   12.977 -15.188   9.473
ATOM   1352 CE   MET B   46   13.566 -16.690   8.775
ATOM   1353 N   ILE B   47   11.933 -11.379   13.030
ATOM   1354 H   ILE B   47   12.327 -10.991   12.196
ATOM   1355 CA   ILE B   47   10.971 -10.568   13.797
ATOM   1356 C   ILE B   47   9.761 -10.233   12.962
ATOM   1357 O   ILE B   47   9.819 -10.048   11.731
ATOM   1358 CB   ILE B   47   11.608   -9.294   14.385
ATOM   1359 CG1 ILE B   47   12.345   -8.459   13.318
ATOM   1360 CG2 ILE B   47   12.542   -9.638   15.494
ATOM   1361 CD1 ILE B   47   12.789   -7.123   13.851
ATOM   1362 N   GLY B   48   8.557 -10.136   13.558
ATOM   1363 H   GLY B   48   8.484 -10.249   14.549
ATOM   1364 CA   GLY B   48   7.365   -9.872   12.800
ATOM   1365 C   GLY B   48   6.826   -8.512   13.141
ATOM   1366 O   GLY B   48   7.136   -7.832   14.149
ATOM   1367 N   GLY B   49   5.940   -8.027   12.306
ATOM   1368 H   GLY B   49   5.668   -8.562   11.506
ATOM   1369 CA   GLY B   49   5.336   -6.745   12.493
ATOM   1370 C   GLY B   49   4.082   -6.786   11.674
ATOM   1371 O   GLY B   49   3.561   -7.847   11.273
ATOM   1372 N   ILE B   50   3.531   -5.634   11.315
ATOM   1373 H   ILE B   50   4.015   -4.777   11.492
ATOM   1374 CA   ILE B   50   2.247   -5.573   10.673
ATOM   1375 C   ILE B   50   2.118   -6.456   9.420
ATOM   1376 O   ILE B   50   1.175   -7.253   9.215
ATOM   1377 CB   ILE B   50   1.982   -4.071   10.391
ATOM   1378 CG1 ILE B   50   1.005   -3.539   11.396
ATOM   1379 CG2 ILE B   50   1.610   -3.739   8.922
ATOM   1380 CD1 ILE B   50   -0.391   -4.077   11.252
ATOM   1381 N   GLY B   51   3.113   -6.410   8.519
ATOM   1382 H   GLY B   51   3.957   -5.920   8.737
ATOM   1383 CA   GLY B   51   2.926   -7.075   7.259
ATOM   1384 C   GLY B   51   3.671   -8.391   7.077
ATOM   1385 O   GLY B   51   3.716   -8.945   5.973
ATOM   1386 N   GLY B   52   4.296   -8.982   8.116
ATOM   1387 H   GLY B   52   4.227   -8.580   9.029
ATOM   1388 CA   GLY B   52   5.053 -10.190   7.874
ATOM   1389 C   GLY B   52   6.334 -10.178   8.678
ATOM   1390 O   GLY B   52   6.519   -9.421   9.657
ATOM   1391 N   PHE B   53   7.325 -11.015   8.343
ATOM   1392 H   PHE B   53   7.227 -11.603   7.540
ATOM   1393 CA   PHE B   53   8.542 -11.096   9.110
ATOM   1394 C   PHE B   53   9.727 -10.584   8.315
ATOM   1395 O   PHE B   53   9.780 -10.618   7.075
ATOM   1396 CB   PHE B   53   8.804 -12.555   9.542
ATOM   1397 CG   PHE B   53   7.850 -13.023   10.592
ATOM   1398 CD1 PHE B   53   6.513 -13.277   10.279
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## FIG. 11 A-24

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Sheet 26 of 33
Title: Use of Computationally Derived Protein Structures of Genetic
Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
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Filed: 11/10/00     Attorney Docket No. 24737-1906C

| ATOM | 1399 | CD2 | PHE | B | 53 | 8.279 | -13.192 | 11.918 |
|------|------|-----|-----|---|----|--------|---------|--------|
| ATOM | 1400 | CE1 | PHE | B | 53 | 5.620 | -13.697 | 11.253 |
| ATOM | 1401 | CE2 | PHE | B | 53 | 7.382 | -13.615 | 12.903 |
| ATOM | 1402 | CZ | PHE | B | 53 | 6.052 | -13.868 | 12.574 |
| ATOM | 1403 | N | ILE | B | 54 | 10.758 | -10.126 | 8.985 |
| ATOM | 1404 | H | ILE | B | 54 | 10.665 | -9.922 | 9.960 |
| ATOM | 1405 | CA | ILE | B | 54 | 12.029 | -9.910 | 8.338 |
| ATOM | 1406 | C | ILE | B | 54 | 13.089 | -10.648 | 9.134 |
| ATOM | 1407 | O | ILE | B | 54 | 12.952 | -11.006 | 10.325 |
| ATOM | 1408 | CB | ILE | B | 54 | 12.390 | -8.444 | 8.236 |
| ATOM | 1409 | CG1 | ILE | B | 54 | 12.386 | -7.775 | 9.611 |
| ATOM | 1410 | CG2 | ILE | B | 54 | 11.460 | -7.770 | 7.218 |
| ATOM | 1411 | CD1 | ILE | B | 54 | 13.113 | -6.438 | 9.590 |
| ATOM | 1412 | N | LYS | B | 55 | 14.272 | -10.852 | 8.523 |
| ATOM | 1413 | H | LYS | B | 55 | 14.383 | -10.599 | 7.562 |
| ATOM | 1414 | CA | LYS | B | 55 | 15.403 | -11.431 | 9.216 |
| ATOM | 1415 | C | LYS | B | 55 | 16.274 | -10.324 | 9.732 |
| ATOM | 1416 | O | LYS | B | 55 | 16.620 | -9.328 | 9.047 |
| ATOM | 1417 | CB | LYS | B | 55 | 16.222 | -12.237 | 8.245 |
| ATOM | 1418 | CG | LYS | B | 55 | 15.638 | -13.596 | 8.063 |
| ATOM | 1419 | CD | LYS | B | 55 | 16.299 | -14.348 | 6.953 |
| ATOM | 1420 | CE | LYS | B | 55 | 15.311 | -14.520 | 5.813 |
| ATOM | 1421 | NZ | LYS | B | 55 | 15.757 | -15.577 | 4.897 |
| ATOM | 1422 | 1HZ | LYS | B | 55 | 15.095 | -15.676 | 4.154 |
| ATOM | 1423 | 3HZ | LYS | B | 55 | 15.830 | -16.441 | 5.395 |
| ATOM | 1424 | 2HZ | LYS | B | 55 | 16.650 | -15.334 | 4.518 |
| ATOM | 1425 | N | VAL | B | 56 | 16.880 | -10.547 | 10.910 |
| ATOM | 1426 | H | VAL | B | 56 | 16.741 | -11.418 | 11.382 |
| ATOM | 1427 | CA | VAL | B | 56 | 17.732 | -9.578 | 11.534 |
| ATOM | 1428 | C | VAL | B | 56 | 18.884 | -10.304 | 12.184 |
| ATOM | 1429 | O | VAL | B | 56 | 18.884 | -11.539 | 12.367 |
| ATOM | 1430 | CB | VAL | B | 56 | 16.912 | -8.819 | 12.609 |
| ATOM | 1431 | CG1 | VAL | B | 56 | 15.865 | -7.943 | 11.921 |
| ATOM | 1432 | CG2 | VAL | B | 56 | 16.215 | -9.788 | 13.599 |
| ATOM | 1433 | N | ARG | B | 57 | 19.958 | -9.593 | 12.591 |
| ATOM | 1434 | H | ARG | B | 57 | 20.030 | -8.624 | 12.353 |
| ATOM | 1435 | CA | ARG | B | 57 | 21.050 | -10.193 | 13.386 |
| ATOM | 1436 | C | ARG | B | 57 | 20.963 | -9.608 | 14.804 |
| ATOM | 1437 | O | ARG | B | 57 | 20.814 | -8.395 | 15.053 |
| ATOM | 1438 | CB | ARG | B | 57 | 22.426 | -9.873 | 12.817 |
| ATOM | 1439 | CG | ARG | B | 57 | 22.664 | -10.437 | 11.439 |
| ATOM | 1440 | CD | ARG | B | 57 | 24.012 | -10.065 | 10.899 |
| ATOM | 1441 | NE | ARG | B | 57 | 24.280 | -10.697 | 9.617 |
| ATOM | 1442 | HE | ARG | B | 57 | 23.592 | -11.323 | 9.250 |
| ATOM | 1443 | CZ | ARG | B | 57 | 25.392 | -10.478 | 8.921 |
| ATOM | 1444 | NH1 | ARG | B | 57 | 26.337 | -9.650 | 9.353 |
| ATOM | 1445 | 2HH1 | ARG | B | 57 | 26.223 | -9.171 | 10.224 |
| ATOM | 1446 | 1HH1 | ARG | B | 57 | 27.163 | -9.505 | 8.808 |
| ATOM | 1447 | NH2 | ARG | B | 57 | 25.561 | -11.104 | 7.760 |
| ATOM | 1448 | 1HH2 | ARG | B | 57 | 26.392 | -10.950 | 7.225 |
| ATOM | 1449 | 2HH2 | ARG | B | 57 | 24.857 | -11.729 | 7.422 |
| ATOM | 1450 | N | GLN | B | 58 | 20.997 | -10.489 | 15.832 |
| ATOM | 1451 | H | GLN | B | 58 | 21.176 | -11.456 | 15.650 |
| ATOM | 1452 | CA | GLN | B | 58 | 20.780 | -10.072 | 17.206 |
| ATOM | 1453 | C | GLN | B | 58 | 22.108 | -9.886 | 17.882 |
| ATOM | 1454 | O | GLN | B | 58 | 22.918 | -10.815 | 18.038 |

# FIG. I I A-25
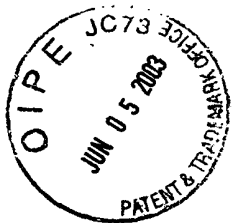
Heller Ehrman White & McAuliffe, LLP
Sheet 27 of 33
Title: Use of Computationally Derived Protein Structures of Genetic
Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
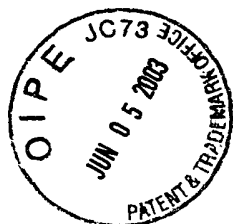Serial No.: 09/709,905      Applicants: Ramnarayan *et al.*
Filed: 11/10/00    Attorney Docket No. 24737-1906C

| | | | | | | | |
|------|------|------|-----|---|---|---------|---------|---------|
| ATOM | 1455 | CB   | GLN | B | 58 | 20.051 | -11.190 | 17.932 |
| ATOM | 1456 | CG   | GLN | B | 58 | 19.765 | -10.845 | 19.366 |
| ATOM | 1457 | CD   | GLN | B | 58 | 19.179 | -12.003 | 20.112 |
| ATOM | 1458 | OE1  | GLN | B | 58 | 19.712 | -12.472 | 21.101 |
| ATOM | 1459 | NE2  | GLN | B | 58 | 18.055 | -12.476 | 19.623 |
| ATOM | 1460 | 1HE2 | GLN | B | 58 | 17.598 | -13.249 | 20.063 |
| ATOM | 1461 | 2HE2 | GLN | B | 58 | 17.647 | -12.066 | 18.807 |
| ATOM | 1462 | N    | TYR | B | 59 | 22.416 | -8.692 | 18.422 |
| ATOM | 1463 | H    | TYR | B | 59 | 21.788 | -7.921 | 18.311 |
| ATOM | 1464 | CA   | TYR | B | 59 | 23.631 | -8.486 | 19.161 |
| ATOM | 1465 | C    | TYR | B | 59 | 23.244 | -8.290 | 20.607 |
| ATOM | 1466 | O    | TYR | B | 59 | 22.178 | -7.728 | 20.927 |
| ATOM | 1467 | CB   | TYR | B | 59 | 24.387 | -7.241 | 18.653 |
| ATOM | 1468 | CG   | TYR | B | 59 | 24.271 | -7.075 | 17.149 |
| ATOM | 1469 | CD1  | TYR | B | 59 | 23.045 | -7.242 | 16.494 |
| ATOM | 1470 | CD2  | TYR | B | 59 | 25.385 | -6.753 | 16.374 |
| ATOM | 1471 | CE1  | TYR | B | 59 | 22.939 | -7.093 | 15.112 |
| ATOM | 1472 | CE2  | TYR | B | 59 | 25.291 | -6.603 | 14.995 |
| ATOM | 1473 | CZ   | TYR | B | 59 | 24.068 | -6.774 | 14.365 |
| ATOM | 1474 | OH   | TYR | B | 59 | 24.018 | -6.620 | 13.010 |
| ATOM | 1475 | HH   | TYR | B | 59 | 24.926 | -6.394 | 12.658 |
| ATOM | 1476 | N    | ASP | B | 60 | 24.010 | -8.785 | 21.596 |
| ATOM | 1477 | H    | ASP | B | 60 | 24.852 | -9.276 | 21.372 |
| ATOM | 1478 | CA   | ASP | B | 60 | 23.644 | -8.624 | 22.992 |
| ATOM | 1479 | C    | ASP | B | 60 | 24.556 | -7.595 | 23.615 |
| ATOM | 1480 | O    | ASP | B | 60 | 25.654 | -7.261 | 23.125 |
| ATOM | 1481 | CB   | ASP | B | 60 | 23.789 | -9.920 | 23.777 |
| ATOM | 1482 | CG   | ASP | B | 60 | 22.803 | -10.960 | 23.332 |
| ATOM | 1483 | OD1  | ASP | B | 60 | 21.619 | -10.634 | 23.032 |
| ATOM | 1484 | OD2  | ASP | B | 60 | 23.208 | -12.126 | 23.273 |
| ATOM | 1485 | N    | GLN | B | 61 | 24.156 | -7.022 | 24.774 |
| ATOM | 1486 | H    | GLN | B | 61 | 23.252 | -7.234 | 25.146 |
| ATOM | 1487 | CA   | GLN | B | 61 | 25.011 | -6.086 | 25.519 |
| ATOM | 1488 | C    | GLN | B | 61 | 25.411 | -4.866 | 24.746 |
| ATOM | 1489 | O    | GLN | B | 61 | 26.560 | -4.382 | 24.832 |
| ATOM | 1490 | CB   | GLN | B | 61 | 26.269 | -6.763 | 26.028 |
| ATOM | 1491 | CG   | GLN | B | 61 | 26.020 | -8.038 | 26.753 |
| ATOM | 1492 | CD   | GLN | B | 61 | 25.714 | -7.766 | 28.185 |
| ATOM | 1493 | OE1  | GLN | B | 61 | 24.572 | -7.455 | 28.548 |
| ATOM | 1494 | NE2  | GLN | B | 61 | 26.744 | -7.844 | 29.014 |
| ATOM | 1495 | 1HE2 | GLN | B | 61 | 26.620 | -7.675 | 29.992 |
| ATOM | 1496 | 2HE2 | GLN | B | 61 | 27.654 | -8.073 | 28.669 |
| ATOM | 1497 | N    | ILE | B | 62 | 24.539 | -4.257 | 23.933 |
| ATOM | 1498 | H    | ILE | B | 62 | 23.628 | -4.648 | 23.801 |
| ATOM | 1499 | CA   | ILE | B | 62 | 24.878 | -3.047 | 23.238 |
| ATOM | 1500 | C    | ILE | B | 62 | 24.571 | -1.885 | 24.144 |
| ATOM | 1501 | O    | ILE | B | 62 | 23.515 | -1.819 | 24.819 |
| ATOM | 1502 | CB   | ILE | B | 62 | 24.097 | -2.922 | 21.912 |
| ATOM | 1503 | CG1  | ILE | B | 62 | 24.310 | -4.170 | 21.094 |
| ATOM | 1504 | CG2  | ILE | B | 62 | 24.568 | -1.709 | 21.067 |
| ATOM | 1505 | CD1  | ILE | B | 62 | 25.794 | -4.479 | 20.878 |
| ATOM | 1506 | N    | LEU | B | 63 | 25.485 | -0.912 | 24.304 |
| ATOM | 1507 | H    | LEU | B | 63 | 26.403 | -1.028 | 23.926 |
| ATOM | 1508 | CA   | LEU | B | 63 | 25.192 | 0.322 | 25.015 |
| ATOM | 1509 | C    | LEU | B | 63 | 24.630 | 1.296 | 24.030 |
| ATOM | 1510 | O    | LEU | B | 63 | 25.239 | 1.658 | 22.995 |

# FIG. 11A-26

Heller Ehrman White & McAuliffe, LLP
Sheet 28 of 33
Title: Use of Computationally Derived Protein Structures of Genetic
Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
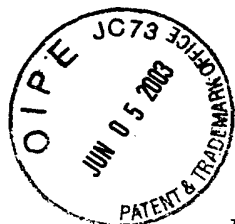Serial No.: 09/709,905        Applicants: Ramnarayan et al.
Filed: 11/10/00    Attorney Docket No. 24737-1906C

| ATOM | 1511 | CB  | LEU | B | 63 | 26.436 | 0.970  | 25.590 |
|------|------|-----|-----|---|----|--------|--------|--------|
| ATOM | 1512 | CG  | LEU | B | 63 | 26.186 | 2.358  | 26.226 |
| ATOM | 1513 | CD1 | LEU | B | 63 | 25.486 | 2.261  | 27.576 |
| ATOM | 1514 | CD2 | LEU | B | 63 | 27.468 | 3.162  | 26.382 |
| ATOM | 1515 | N   | ILE | B | 64 | 23.492 | 1.946  | 24.358 |
| ATOM | 1516 | H   | ILE | B | 64 | 22.958 | 1.643  | 25.148 |
| ATOM | 1517 | CA  | ILE | B | 64 | 23.003 | 3.068  | 23.617 |
| ATOM | 1518 | C   | ILE | B | 64 | 22.872 | 4.194  | 24.612 |
| ATOM | 1519 | O   | ILE | B | 64 | 22.915 | 4.007  | 25.846 |
| ATOM | 1520 | CB  | ILE | B | 64 | 21.634 | 2.701  | 22.989 |
| ATOM | 1521 | CG1 | ILE | B | 64 | 21.825 | 1.521  | 22.029 |
| ATOM | 1522 | CG2 | ILE | B | 64 | 20.982 | 3.894  | 22.246 |
| ATOM | 1523 | CD1 | ILE | B | 64 | 20.593 | 1.096  | 21.260 |
| ATOM | 1524 | N   | GLU | B | 65 | 22.803 | 5.460  | 24.172 |
| ATOM | 1525 | H   | GLU | B | 65 | 23.013 | 5.664  | 23.216 |
| ATOM | 1526 | CA  | GLU | B | 65 | 22.432 | 6.551  | 25.037 |
| ATOM | 1527 | C   | GLU | B | 65 | 21.242 | 7.194  | 24.373 |
| ATOM | 1528 | O   | GLU | B | 65 | 21.312 | 7.729  | 23.257 |
| ATOM | 1529 | CB  | GLU | B | 65 | 23.497 | 7.615  | 25.131 |
| ATOM | 1530 | CG  | GLU | B | 65 | 24.787 | 7.196  | 25.761 |
| ATOM | 1531 | CD  | GLU | B | 65 | 25.694 | 8.385  | 26.076 |
| ATOM | 1532 | OE1 | GLU | B | 65 | 25.170 | 9.510  | 26.311 |
| ATOM | 1533 | OE2 | GLU | B | 65 | 26.938 | 8.200  | 26.092 |
| ATOM | 1534 | N   | ILE | B | 66 | 20.078 | 7.240  | 25.035 |
| ATOM | 1535 | H   | ILE | B | 66 | 20.010 | 6.835  | 25.947 |
| ATOM | 1536 | CA  | ILE | B | 66 | 18.907 | 7.865  | 24.462 |
| ATOM | 1537 | C   | ILE | B | 66 | 18.777 | 9.195  | 25.145 |
| ATOM | 1538 | O   | ILE | B | 66 | 18.591 | 9.303  | 26.379 |
| ATOM | 1539 | CB  | ILE | B | 66 | 17.713 | 6.995  | 24.790 |
| ATOM | 1540 | CG1 | ILE | B | 66 | 17.916 | 5.583  | 24.335 |
| ATOM | 1541 | CG2 | ILE | B | 66 | 16.405 | 7.544  | 24.177 |
| ATOM | 1542 | CD1 | ILE | B | 66 | 16.888 | 4.677  | 24.884 |
| ATOM | 1543 | N   | CYS | B | 67 | 18.965 | 10.325 | 24.437 |
| ATOM | 1544 | H   | CYS | B | 67 | 19.201 | 10.268 | 23.467 |
| ATOM | 1545 | CA  | CYS | B | 67 | 18.833 | 11.663 | 25.049 |
| ATOM | 1546 | C   | CYS | B | 67 | 19.637 | 11.781 | 26.319 |
| ATOM | 1547 | O   | CYS | B | 67 | 19.235 | 12.400 | 27.328 |
| ATOM | 1548 | CB  | CYS | B | 67 | 17.387 | 12.023 | 25.319 |
| ATOM | 1549 | SG  | CYS | B | 67 | 16.407 | 12.259 | 23.821 |
| ATOM | 1550 | N   | GLY | B | 68 | 20.830 | 11.180 | 26.383 |
| ATOM | 1551 | H   | GLY | B | 68 | 21.158 | 10.646 | 25.604 |
| ATOM | 1552 | CA  | GLY | B | 68 | 21.654 | 11.288 | 27.558 |
| ATOM | 1553 | C   | GLY | B | 68 | 21.464 | 10.185 | 28.584 |
| ATOM | 1554 | O   | GLY | B | 68 | 22.174 | 10.128 | 29.606 |
| ATOM | 1555 | N   | HIS | B | 69 | 20.513 | 9.255  | 28.425 |
| ATOM | 1556 | H   | HIS | B | 69 | 19.924 | 9.282  | 27.618 |
| ATOM | 1557 | CA  | HIS | B | 69 | 20.304 | 8.199  | 29.391 |
| ATOM | 1558 | C   | HIS | B | 69 | 20.861 | 6.936  | 28.811 |
| ATOM | 1559 | O   | HIS | B | 69 | 20.589 | 6.560  | 27.647 |
| ATOM | 1560 | CB  | HIS | B | 69 | 18.832 | 7.992  | 29.654 |
| ATOM | 1561 | CG  | HIS | B | 69 | 18.175 | 9.203  | 30.223 |
| ATOM | 1562 | ND1 | HIS | B | 69 | 17.504 | 9.195  | 31.435 |
| ATOM | 1563 | HD1 | HIS | B | 69 | 17.383 | 8.402  | 32.032 |
| ATOM | 1564 | CD2 | HIS | B | 69 | 18.122 | 10.470 | 29.729 |
| ATOM | 1565 | CE1 | HIS | B | 69 | 17.070 | 10.429 | 31.626 |
| ATOM | 1566 | NE2 | HIS | B | 69 | 17.410 | 11.240 | 30.635 |

FIG. 11A-27
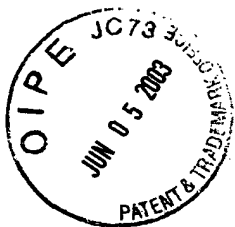
| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1567 | N | LYS | B | 70 | 21.751 | 6.217 | 29.499 |
| ATOM | 1568 | H | LYS | B | 70 | 22.025 | 6.512 | 30.414 |
| ATOM | 1569 | CA | LYS | B | 70 | 22.326 | 5.020 | 28.945 |
| ATOM | 1570 | C | LYS | B | 70 | 21.386 | 3.854 | 29.145 |
| ATOM | 1571 | O | LYS | B | 70 | 20.627 | 3.725 | 30.120 |
| ATOM | 1572 | CB | LYS | B | 70 | 23.613 | 4.678 | 29.663 |
| ATOM | 1573 | CG | LYS | B | 70 | 24.694 | 5.655 | 29.379 |
| ATOM | 1574 | CD | LYS | B | 70 | 25.739 | 5.524 | 30.444 |
| ATOM | 1575 | CE | LYS | B | 70 | 27.048 | 6.090 | 30.011 |
| ATOM | 1576 | NZ | LYS | B | 70 | 26.948 | 7.548 | 30.000 |
| ATOM | 1577 | 1HZ | LYS | B | 70 | 27.821 | 7.940 | 29.711 |
| ATOM | 1578 | 3HZ | LYS | B | 70 | 26.725 | 7.874 | 30.919 |
| ATOM | 1579 | 2HZ | LYS | B | 70 | 26.230 | 7.828 | 29.363 |
| ATOM | 1580 | N | ALA | B | 71 | 21.512 | 2.849 | 28.284 |
| ATOM | 1581 | H | ALA | B | 71 | 22.141 | 2.934 | 27.512 |
| ATOM | 1582 | CA | ALA | B | 71 | 20.762 | 1.630 | 28.432 |
| ATOM | 1583 | C | ALA | B | 71 | 21.629 | 0.576 | 27.805 |
| ATOM | 1584 | O | ALA | B | 71 | 22.463 | 0.830 | 26.912 |
| ATOM | 1585 | CB | ALA | B | 71 | 19.452 | 1.726 | 27.737 |
| ATOM | 1586 | N | ILE | B | 72 | 21.547 | -0.681 | 28.237 |
| ATOM | 1587 | H | ILE | B | 72 | 20.864 | -0.925 | 28.926 |
| ATOM | 1588 | CA | ILE | B | 72 | 22.424 | -1.698 | 27.730 |
| ATOM | 1589 | C | ILE | B | 72 | 21.615 | -2.938 | 27.462 |
| ATOM | 1590 | O | ILE | B | 72 | 20.909 | -3.490 | 28.330 |
| ATOM | 1591 | CB | ILE | B | 72 | 23.524 | -1.999 | 28.737 |
| ATOM | 1592 | CG1 | ILE | B | 72 | 24.322 | -0.735 | 29.090 |
| ATOM | 1593 | CG2 | ILE | B | 72 | 24.442 | -3.037 | 28.153 |
| ATOM | 1594 | CD1 | ILE | B | 72 | 25.374 | -1.012 | 30.163 |
| ATOM | 1595 | N | GLY | B | 73 | 21.609 | -3.446 | 26.235 |
| ATOM | 1596 | H | GLY | B | 73 | 22.204 | -3.054 | 25.534 |
| ATOM | 1597 | CA | GLY | B | 73 | 20.707 | -4.545 | 26.062 |
| ATOM | 1598 | C | GLY | B | 73 | 20.828 | -5.084 | 24.663 |
| ATOM | 1599 | O | GLY | B | 73 | 21.754 | -4.831 | 23.863 |
| ATOM | 1600 | N | THR | B | 74 | 19.856 | -5.905 | 24.271 |
| ATOM | 1601 | H | THR | B | 74 | 19.086 | -6.088 | 24.882 |
| ATOM | 1602 | CA | THR | B | 74 | 19.869 | -6.548 | 22.988 |
| ATOM | 1603 | C | THR | B | 74 | 19.363 | -5.590 | 21.931 |
| ATOM | 1604 | O | THR | B | 74 | 18.338 | -4.870 | 22.053 |
| ATOM | 1605 | CB | THR | B | 74 | 19.011 | -7.801 | 23.074 |
| ATOM | 1606 | OG1 | THR | B | 74 | 19.611 | -8.683 | 24.013 |
| ATOM | 1607 | HG1 | THR | B | 74 | 19.068 | -9.519 | 24.092 |
| ATOM | 1608 | CG2 | THR | B | 74 | 18.817 | -8.496 | 21.705 |
| ATOM | 1609 | N | VAL | B | 75 | 20.028 | -5.620 | 20.762 |
| ATOM | 1610 | H | VAL | B | 75 | 20.835 | -6.203 | 20.666 |
| ATOM | 1611 | CA | VAL | B | 75 | 19.630 | -4.837 | 19.611 |
| ATOM | 1612 | C | VAL | B | 75 | 19.600 | -5.771 | 18.426 |
| ATOM | 1613 | O | VAL | B | 75 | 20.444 | -6.673 | 18.230 |
| ATOM | 1614 | CB | VAL | B | 75 | 20.667 | -3.712 | 19.395 |
| ATOM | 1615 | CG1 | VAL | B | 75 | 20.473 | -3.002 | 18.046 |
| ATOM | 1616 | CG2 | VAL | B | 75 | 20.679 | -2.708 | 20.567 |
| ATOM | 1617 | N | LEU | B | 76 | 18.557 | -5.647 | 17.565 |
| ATOM | 1618 | H | LEU | B | 76 | 17.822 | -5.000 | 17.767 |
| ATOM | 1619 | CA | LEU | B | 76 | 18.444 | -6.427 | 16.324 |
| ATOM | 1620 | C | LEU | B | 76 | 18.736 | -5.487 | 15.144 |
| ATOM | 1621 | O | LEU | B | 76 | 18.239 | -4.343 | 15.040 |
| ATOM | 1622 | CB | LEU | B | 76 | 17.028 | -7.021 | 16.158 |

## FIG. I I A- 28

Heller Ehrman White & McAuliffe, LLP
Sheet 30 of 33
Title: Use of Computationally Derived Protein Structures of Genetic
Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
Serial No.: 09/709,905      Applicants: Ramnarayan *et al.*
Filed: 11/10/00      Attorney Docket No. 24737-1906C

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ATOM   1623 CG   LEU B 76   16.427   -7.612   17.449
ATOM   1624 CD1 LEU B 76   14.992   -8.075   17.263
ATOM   1625 CD2 LEU B 76   17.266   -8.758   18.019
ATOM   1626 N   VAL B 77   19.607   -5.900   14.222
ATOM   1627 H   VAL B 77   19.985   -6.824   14.276
ATOM   1628 CA   VAL B 77   20.027   -5.042   13.133
ATOM   1629 C   VAL B 77   19.570   -5.662   11.842
ATOM   1630 O   VAL B 77   19.678   -6.883   11.598
ATOM   1631 CB   VAL B 77   21.563   -4.905   13.191
ATOM   1632 CG1 VAL B 77   22.129   -4.202   11.944
ATOM   1633 CG2 VAL B 77   22.030   -4.166   14.470
ATOM   1634 N   GLY B 78   18.978   -4.915   10.943
ATOM   1635 H   GLY B 78   18.841   -3.941   11.121
ATOM   1636 CA   GLY B 78   18.523   -5.475   9.705
ATOM   1637 C   GLY B 78   18.019   -4.338   8.874
ATOM   1638 O   GLY B 78   18.130   -3.142   9.223
ATOM   1639 N   PRO B 79   17.408   -4.596   7.722
ATOM   1640 CA   PRO B 79   16.954   -3.535   6.834
ATOM   1641 C   PRO B 79   15.635   -2.872   7.280
ATOM   1642 O   PRO B 79   14.609   -2.877   6.565
ATOM   1643 CB   PRO B 79   16.804   -4.274   5.492
ATOM   1644 CG   PRO B 79   16.463   -5.712   5.881
ATOM   1645 CD   PRO B 79   17.159   -5.959   7.189
ATOM   1646 N   THR B 80   15.574   -2.247   8.458
ATOM   1647 H   THR B 80   16.374   -2.242   9.058
ATOM   1648 CA   THR B 80   14.364   -1.583   8.865
ATOM   1649 C   THR B 80   14.312   -0.189   8.228
ATOM   1650 O   THR B 80   15.349   0.471   8.001
ATOM   1651 CB   THR B 80   14.250   -1.512   10.410
ATOM   1652 OG1 THR B 80   13.079   -0.802   10.806
ATOM   1653 HG1 THR B 80   13.022   -0.766   11.804
ATOM   1654 CG2 THR B 80   15.519   -0.901   11.062
ATOM   1655 N   PRO B 81   13.137   0.354   7.885
ATOM   1656 CA   PRO B 81   13.036   1.747   7.379
ATOM   1657 C   PRO B 81   13.363   2.732   8.484
ATOM   1658 O   PRO B 81   13.791   3.880   8.250
ATOM   1659 CB   PRO B 81   11.548   1.912   6.982
ATOM   1660 CG   PRO B 81   10.819   0.674   7.488
ATOM   1661 CD   PRO B 81   11.854   -0.387   7.797
ATOM   1662 N   VAL B 82   13.197   2.368   9.772
ATOM   1663 H   VAL B 82   12.940   1.427   9.992
ATOM   1664 CA   VAL B 82   13.380   3.306   10.885
ATOM   1665 C   VAL B 82   14.160   2.668   12.010
ATOM   1666 O   VAL B 82   14.045   1.465   12.293
ATOM   1667 CB   VAL B 82   11.996   3.695   11.431
ATOM   1668 CG1 VAL B 82   12.055   4.961   12.269
ATOM   1669 CG2 VAL B 82   10.958   3.857   10.318
ATOM   1670 N   ASN B 83   14.963   3.422   12.775
ATOM   1671 H   ASN B 83   15.147   4.370   12.516
ATOM   1672 CA   ASN B 83   15.550   2.846   13.967
ATOM   1673 C   ASN B 83   14.481   2.874   15.022
ATOM   1674 O   ASN B 83   13.814   3.903   15.294
ATOM   1675 CB   ASN B 83   16.743   3.639   14.472
ATOM   1676 CG   ASN B 83   17.935   3.574   13.570
ATOM   1677 OD1 ASN B 83   18.409   2.511   13.167
ATOM   1678 ND2 ASN B 83   18.439   4.735   13.238
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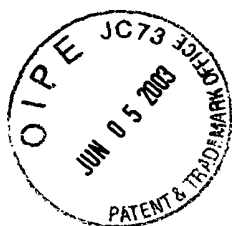
## FIG. 11A-29
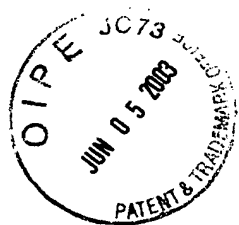
Heller Ehrman White & McAuliffe, LLP
Sheet 31 of 33
Title: Use of Computationally Derived Protein Structures of Genetic
Polymorphisms in Pharmacogenomics for Drug Design and Clinical Applications
Serial No.: 09/709,905        Applicants: Ramnarayan *et al.*
Filed: 11/10/00     Attorney Docket No. 24737-1906C

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1679 | 2HD2 | ASN | B | 83 | 19.237 | 4.786 | 12.638 |
| ATOM | 1680 | 1HD2 | ASN | B | 83 | 18.030 | 5.580 | 13.582 |
| ATOM | 1681 | N | ILE | B | 84 | 14.225 | 1.749 | 15.711 |
| ATOM | 1682 | H | ILE | B | 84 | 14.791 | 0.938 | 15.564 |
| ATOM | 1683 | CA | ILE | B | 84 | 13.154 | 1.658 | 16.667 |
| ATOM | 1684 | C | ILE | B | 84 | 13.740 | 1.317 | 18.020 |
| ATOM | 1685 | O | ILE | B | 84 | 14.428 | 0.300 | 18.223 |
| ATOM | 1686 | CB | ILE | B | 84 | 12.214 | 0.517 | 16.260 |
| ATOM | 1687 | CG1 | ILE | B | 84 | 11.656 | 0.759 | 14.849 |
| ATOM | 1688 | CG2 | ILE | B | 84 | 11.128 | 0.247 | 17.315 |
| ATOM | 1689 | CD1 | ILE | B | 84 | 10.770 | -0.359 | 14.291 |
| ATOM | 1690 | N | ILE | B | 85 | 13.483 | 2.157 | 19.051 |
| ATOM | 1691 | H | ILE | B | 85 | 13.028 | 3.030 | 18.877 |
| ATOM | 1692 | CA | ILE | B | 85 | 13.846 | 1.834 | 20.408 |
| ATOM | 1693 | C | ILE | B | 85 | 12.596 | 1.254 | 21.085 |
| ATOM | 1694 | O | ILE | B | 85 | 11.536 | 1.903 | 21.267 |
| ATOM | 1695 | CB | ILE | B | 85 | 14.308 | 3.115 | 21.137 |
| ATOM | 1696 | CG1 | ILE | B | 85 | 15.447 | 3.826 | 20.395 |
| ATOM | 1697 | CG2 | ILE | B | 85 | 14.673 | 2.840 | 22.589 |
| ATOM | 1698 | CD1 | ILE | B | 85 | 16.730 | 3.053 | 20.263 |
| ATOM | 1699 | N | GLY | B | 86 | 12.617 | -0.052 | 21.422 |
| ATOM | 1700 | H | GLY | B | 86 | 13.439 | -0.595 | 21.251 |
| ATOM | 1701 | CA | GLY | B | 86 | 11.481 | -0.702 | 22.028 |
| ATOM | 1702 | C | GLY | B | 86 | 11.557 | -0.748 | 23.538 |
| ATOM | 1703 | O | GLY | B | 86 | 12.412 | -0.165 | 24.238 |
| ATOM | 1704 | N | ARG | B | 87 | 10.614 | -1.489 | 24.149 |
| ATOM | 1705 | H | ARG | B | 87 | 10.012 | -2.072 | 23.604 |
| ATOM | 1706 | CA | ARG | B | 87 | 10.442 | -1.468 | 25.584 |
| ATOM | 1707 | C | ARG | B | 87 | 11.627 | -2.021 | 26.326 |
| ATOM | 1708 | O | ARG | B | 87 | 11.911 | -1.666 | 27.495 |
| ATOM | 1709 | CB | ARG | B | 87 | 9.200 | -2.271 | 25.949 |
| ATOM | 1710 | CG | ARG | B | 87 | 7.951 | -1.960 | 25.161 |
| ATOM | 1711 | CD | ARG | B | 87 | 6.956 | -3.074 | 25.219 |
| ATOM | 1712 | NE | ARG | B | 87 | 5.906 | -2.933 | 24.205 |
| ATOM | 1713 | HE | ARG | B | 87 | 5.790 | -2.039 | 23.772 |
| ATOM | 1714 | CZ | ARG | B | 87 | 5.119 | -3.953 | 23.856 |
| ATOM | 1715 | NH1 | ARG | B | 87 | 5.252 | -5.161 | 24.396 |
| ATOM | 1716 | 2HH1 | ARG | B | 87 | 5.958 | -5.326 | 25.085 |
| ATOM | 1717 | 1HH1 | ARG | B | 87 | 4.646 | -5.905 | 24.113 |
| ATOM | 1718 | NH2 | ARG | B | 87 | 4.180 | -3.751 | 22.939 |
| ATOM | 1719 | 1HH2 | ARG | B | 87 | 3.580 | -4.502 | 22.664 |
| ATOM | 1720 | 2HH2 | ARG | B | 87 | 4.073 | -2.848 | 22.524 |
| ATOM | 1721 | N | ASN | B | 88 | 12.413 | -2.937 | 25.731 |
| ATOM | 1722 | H | ASN | B | 88 | 12.206 | -3.237 | 24.800 |
| ATOM | 1723 | CA | ASN | B | 88 | 13.582 | -3.519 | 26.415 |
| ATOM | 1724 | C | ASN | B | 88 | 14.532 | -2.429 | 26.821 |
| ATOM | 1725 | O | ASN | B | 88 | 15.214 | -2.516 | 27.863 |
| ATOM | 1726 | CB | ASN | B | 88 | 14.285 | -4.605 | 25.559 |
| ATOM | 1727 | CG | ASN | B | 88 | 15.063 | -4.031 | 24.358 |
| ATOM | 1728 | OD1 | ASN | B | 88 | 14.515 | -3.245 | 23.612 |
| ATOM | 1729 | ND2 | ASN | B | 88 | 16.333 | -4.445 | 24.180 |
| ATOM | 1730 | 2HD2 | ASN | B | 88 | 16.875 | -4.099 | 23.414 |
| ATOM | 1731 | 1HD2 | ASN | B | 88 | 16.744 | -5.102 | 24.812 |
| ATOM | 1732 | N | LEU | B | 89 | 14.695 | -1.328 | 26.061 |
| ATOM | 1733 | H | LEU | B | 89 | 14.192 | -1.240 | 25.201 |
| ATOM | 1734 | CA | LEU | B | 89 | 15.597 | -0.234 | 26.452 |

## FIG. 11A-30

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Filed: 11/10/00      Attorney Docket No. 24737-1906C

| ATOM | 1735 | C | LEU | B | 89 | 14.797 | 0.937 | 27.053 |
|------|------|-----|-----|---|----|--------|--------|--------|
| ATOM | 1736 | O | LEU | B | 89 | 15.293 | 1.734 | 27.879 |
| ATOM | 1737 | CB | LEU | B | 89 | 16.421 | 0.232 | 25.236 |
| ATOM | 1738 | CG | LEU | B | 89 | 17.400 | -0.754 | 24.567 |
| ATOM | 1739 | CD1 | LEU | B | 89 | 18.215 | 0.002 | 23.573 |
| ATOM | 1740 | CD2 | LEU | B | 89 | 18.352 | -1.458 | 25.570 |
| ATOM | 1741 | N | LEU | B | 90 | 13.511 | 1.114 | 26.705 |
| ATOM | 1742 | H | LEU | B | 90 | 13.082 | 0.486 | 26.056 |
| ATOM | 1743 | CA | LEU | B | 90 | 12.698 | 2.221 | 27.257 |
| ATOM | 1744 | C | LEU | B | 90 | 12.537 | 2.060 | 28.751 |
| ATOM | 1745 | O | LEU | B | 90 | 12.575 | 3.033 | 29.533 |
| ATOM | 1746 | CB | LEU | B | 90 | 11.311 | 2.258 | 26.628 |
| ATOM | 1747 | CG | LEU | B | 90 | 11.232 | 2.730 | 25.168 |
| ATOM | 1748 | CD1 | LEU | B | 90 | 9.808 | 2.744 | 24.642 |
| ATOM | 1749 | CD2 | LEU | B | 90 | 11.831 | 4.105 | 24.982 |
| ATOM | 1750 | N | THR | B | 91 | 12.315 | 0.843 | 29.271 |
| ATOM | 1751 | H | THR | B | 91 | 12.218 | 0.055 | 28.663 |
| ATOM | 1752 | CA | THR | B | 91 | 12.210 | 0.634 | 30.699 |
| ATOM | 1753 | C | THR | B | 91 | 13.537 | 1.028 | 31.375 |
| ATOM | 1754 | O | THR | B | 91 | 13.575 | 1.525 | 32.518 |
| ATOM | 1755 | CB | THR | B | 91 | 11.893 | -0.843 | 31.028 |
| ATOM | 1756 | OG1 | THR | B | 91 | 12.919 | -1.676 | 30.504 |
| ATOM | 1757 | HG1 | THR | B | 91 | 12.722 | -2.634 | 30.713 |
| ATOM | 1758 | CG2 | THR | B | 91 | 10.599 | -1.285 | 30.418 |
| ATOM | 1759 | N | GLN | B | 92 | 14.705 | 0.852 | 30.732 |
| ATOM | 1760 | H | GLN | B | 92 | 14.707 | 0.497 | 29.797 |
| ATOM | 1761 | CA | GLN | B | 92 | 15.920 | 1.190 | 31.433 |
| ATOM | 1762 | C | GLN | B | 92 | 16.088 | 2.660 | 31.633 |
| ATOM | 1763 | O | GLN | B | 92 | 16.807 | 3.137 | 32.527 |
| ATOM | 1764 | CB | GLN | B | 92 | 17.127 | 0.680 | 30.682 |
| ATOM | 1765 | CG | GLN | B | 92 | 17.076 | -0.805 | 30.517 |
| ATOM | 1766 | CD | GLN | B | 92 | 18.336 | -1.314 | 29.900 |
| ATOM | 1767 | OE1 | GLN | B | 92 | 19.394 | -0.720 | 30.059 |
| ATOM | 1768 | NE2 | GLN | B | 92 | 18.221 | -2.411 | 29.195 |
| ATOM | 1769 | 1HE2 | GLN | B | 92 | 19.022 | -2.813 | 28.751 |
| ATOM | 1770 | 2HE2 | GLN | B | 92 | 17.331 | -2.856 | 29.095 |
| ATOM | 1771 | N | ILE | B | 93 | 15.538 | 3.512 | 30.746 |
| ATOM | 1772 | H | ILE | B | 93 | 15.016 | 3.153 | 29.972 |
| ATOM | 1773 | CA | ILE | B | 93 | 15.693 | 4.937 | 30.899 |
| ATOM | 1774 | C | ILE | B | 93 | 14.522 | 5.549 | 31.698 |
| ATOM | 1775 | O | ILE | B | 93 | 14.438 | 6.773 | 31.940 |
| ATOM | 1776 | CB | ILE | B | 93 | 15.981 | 5.657 | 29.548 |
| ATOM | 1777 | CG1 | ILE | B | 93 | 14.746 | 5.718 | 28.619 |
| ATOM | 1778 | CG2 | ILE | B | 93 | 17.223 | 5.060 | 28.874 |
| ATOM | 1779 | CD1 | ILE | B | 93 | 14.946 | 6.734 | 27.488 |
| ATOM | 1780 | N | GLY | B | 94 | 13.617 | 4.731 | 32.263 |
| ATOM | 1781 | H | GLY | B | 94 | 13.639 | 3.752 | 32.060 |
| ATOM | 1782 | CA | GLY | B | 94 | 12.594 | 5.224 | 33.170 |
| ATOM | 1783 | C | GLY | B | 94 | 11.443 | 5.846 | 32.432 |
| ATOM | 1784 | O | GLY | B | 94 | 10.766 | 6.803 | 32.878 |
| ATOM | 1785 | N | CYS | B | 95 | 11.134 | 5.354 | 31.225 |
| ATOM | 1786 | H | CYS | B | 95 | 11.603 | 4.538 | 30.888 |
| ATOM | 1787 | CA | CYS | B | 95 | 10.134 | 5.969 | 30.381 |
| ATOM | 1788 | C | CYS | B | 95 | 8.750 | 5.512 | 30.764 |
| ATOM | 1789 | O | CYS | B | 95 | 8.478 | 4.309 | 31.006 |
| ATOM | 1790 | CB | CYS | B | 95 | 10.456 | 5.643 | 28.922 |

## FIG. 11A-31

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Filed: 11/10/00      Attorney Docket No. 24737-1906C

| ATOM | 1791 | SG | CYS | B | 95 | 9.426 | 6.512 | 27.764 |
|------|------|-----|-----|---|----|-------|-------|--------|
| ATOM | 1792 | N | THR | B | 96 | 7.778 | 6.444 | 30.764 |
| ATOM | 1793 | H | THR | B | 96 | 8.014 | 7.401 | 30.539 |
| ATOM | 1794 | CA | THR | B | 96 | 6.379 | 6.163 | 31.108 |
| ATOM | 1795 | C | THR | B | 96 | 5.390 | 6.970 | 30.254 |
| ATOM | 1796 | O | THR | B | 96 | 5.567 | 8.171 | 30.066 |
| ATOM | 1797 | CB | THR | B | 96 | 6.111 | 6.439 | 32.604 |
| ATOM | 1798 | OG1 | THR | B | 96 | 6.341 | 7.794 | 32.938 |
| ATOM | 1799 | HG1 | THR | B | 96 | 6.111 | 7.924 | 33.861 |
| ATOM | 1800 | CG2 | THR | B | 96 | 6.938 | 5.566 | 33.554 |
| ATOM | 1801 | N | LEU | B | 97 | 4.302 | 6.321 | 29.809 |
| ATOM | 1802 | H | LEU | B | 97 | 4.216 | 5.332 | 29.997 |
| ATOM | 1803 | CA | LEU | B | 97 | 3.127 | 6.986 | 29.238 |
| ATOM | 1804 | C | LEU | B | 97 | 2.336 | 7.681 | 30.358 |
| ATOM | 1805 | O | LEU | B | 97 | 2.350 | 7.221 | 31.499 |
| ATOM | 1806 | CB | LEU | B | 97 | 2.226 | 5.958 | 28.532 |
| ATOM | 1807 | CG | LEU | B | 97 | 2.860 | 5.279 | 27.300 |
| ATOM | 1808 | CD1 | LEU | B | 97 | 2.101 | 3.986 | 26.957 |
| ATOM | 1809 | CD2 | LEU | B | 97 | 2.842 | 6.216 | 26.085 |
| ATOM | 1810 | N | ASN | B | 98 | 1.637 | 8.777 | 30.024 |
| ATOM | 1811 | H | ASN | B | 98 | 1.662 | 9.086 | 29.063 |
| ATOM | 1812 | CA | ASN | B | 98 | 0.906 | 9.631 | 30.960 |
| ATOM | 1813 | C | ASN | B | 98 | -0.251 | 10.321 | 30.231 |
| ATOM | 1814 | O | ASN | B | 98 | -0.032 | 11.303 | 29.522 |
| ATOM | 1815 | CB | ASN | B | 98 | 1.845 | 10.678 | 31.587 |
| ATOM | 1816 | CG | ASN | B | 98 | 2.783 | 10.077 | 32.634 |
| ATOM | 1817 | OD1 | ASN | B | 98 | 3.926 | 9.739 | 32.335 |
| ATOM | 1818 | ND2 | ASN | B | 98 | 2.297 | 9.942 | 33.870 |
| ATOM | 1819 | 2HD2 | ASN | B | 98 | 2.877 | 9.551 | 34.599 |
| ATOM | 1820 | 1HD2 | ASN | B | 98 | 1.351 | 10.229 | 34.074 |
| ATOM | 1821 | N | LEU | B | 99 | -1.476 | 9.808 | 30.426 |
| ATOM | 1822 | H | LEU | B | 99 | -1.568 | 9.010 | 31.037 |
| ATOM | 1823 | CA | LEU | B | 99 | -2.709 | 10.288 | 29.797 |
| ATOM | 1824 | C | LEU | B | 99 | -3.816 | 10.589 | 30.815 |
| ATOM | 1825 | O | LEU | B | 99 | -3.630 | 10.272 | 32.011 |
| ATOM | 1826 | CB | LEU | B | 99 | -3.146 | 9.340 | 28.657 |
| ATOM | 1827 | CG | LEU | B | 99 | -3.714 | 7.932 | 28.941 |
| ATOM | 1828 | CD1 | LEU | B | 99 | -2.767 | 7.057 | 29.774 |
| ATOM | 1829 | CD2 | LEU | B | 99 | -5.134 | 7.943 | 29.528 |
| ATOM | 1830 | OXT | LEU | B | 99 | -4.842 | 11.156 | 30.376 |
| TER | | | | | | | | |

FIG. II A-32